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Possible Hosts for Quadruply Ionized $3d^N$ Transition Metal Ions: Na_2TiSiO_5, $Y_2SiBe_2O_7$, $Bi_4X_3O_{12}$, and $Bi_{12}XO_{20}$ (X = Si, Ge)

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13. ABSTRACT *(Maximum 200 words)*

This report provides the crystal-field splitting of Cr^{4+} in the host materials Na_2TiSiO_5, $Y_2SiBe_2O_7$, $Bi_4X_3O_{12}$, and $Bi_{12}XO_{20}$. The strength of the crystal field is estimated by evaluating the coefficients of a multipole expansion of the crystal field for the Ti, Si, or Ge site and using empirical values of the radial integrals, $\langle r^4 \rangle$. With the exception of the Ti site in Na_2TiSiO_7, the Si or Ge sites (D_{2d} or S_4 symmetry) are, to a certain degree, approximately tetrahedral. In the material $Bi_{12}XO_{20}$ the X site (Ge or Si) has the cubic symmetry T. Estimated values of the parameters for the quadruply ionized $3d^N$ electronic configurations are given for X = Ge. The energy levels are calculated with and without the spin-orbit interaction. The spin-orbit constant is chosen equal to the free-ion value.

14. SUBJECT TERMS

Cr^{4+}, Na_2TiSiO_5, $Y_2SiBe_2O_7$, $Bi_4Ge_3O_{12}$, $Bi_4Si_3O_{12}$, $Bi_{12}GeO_{20}$, $Bi_{12}SiO_{20}$, V^{4+}, Mn^{4+}, Fe^{4+}, Co^{4+}, Ni^{4+}, Zn^{4+}, Ga^{4+}, optical spectra

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1. Introduction

We have selected six compounds as possible host materials for the study of the optical spectra of the quadruply ionized elements with a $3d^N$ electronic configuration (X^{4+}). Previous hosts for which optical spectra of these ions have been investigated have serious drawbacks to the analysis of the experimental data. Frequently the X^{4+} ion is assumed to enter substitutionally for a triply ionized element of the host, such as Mn^{4+} in yttrium aluminum garnet (YAG) [1]. In such a case the charge compensation generally perturbs the spectra, giving many more lines than should exist for Mn^{4+}. Further, the Mn^{4+} is assumed to go into the C_{3i} site. If it did, the electric dipole transitions would be forbidden and only magnetic dipole transition would be allowed for the zero phonon lines. Thus, the numerous vibrational assisted electric dipole transitions would be as large or larger than the zero phonon lines. Also, in most of the cases reported, the X^{4+} ion replaces a quadruply ionized element of the host, but the site symmetry does not allow electric dipole transitions and the spectra must be sorted out from the numerous vibronics. An additional difficulty arises when the symmetry of the site occupied by the transition metal ion is low, such as C_2 symmetry. Then the number of crystal-field parameters is large, thus requiring a large number of levels of the ion to be determined. In our selection of host materials presented here, we have attempted to avoid some of these difficulties.

Each of the host crystals have either Si^{4+} or Ge^{4+} as a constituent and we assume that under suitable growth conditions a number of X^{4+} ions can replace these ions substitutionally. In all six host crystals, the Si or Ge site has approximately tetrahedral symmetry (either S_4 or D_{2d} symmetry) and in $Bi_{12}XO_{20}$ (X = Ge, Si) the X site has the tetrahedral cubic symmetry, T. In the crystal Na_2TiSiO_5, the lighter X^{4+} ions (V, Cr) might enter the Ti site, which has approximately octahedral symmetry (C_{4v}), but the heavier X^{4+} ions (Ni, Cu) could replace the Si ion, which has approximately tetrahedral symmetry (D_{2d}). In all cases the actual symmetry of the site has a maximum of three crystal-field parameters (B_{20}, B_{40}, and B_{44}) while in $Bi_{12}XO_{20}$ the X site has only one crystal-field parameter (B_{40}). The symmetry of the Ge and Si sites in all these compounds allows electric dipole transitions so that, in general, the electronic transitions would be stronger than the vibronic lines, and identification of the levels would be easier.

In this report, the detailed x-ray data on the six host materials are given along with references to the growth of these crystals. The x-ray data are used to obtain the crystal-field components, A_{kq}, and the monopole components of A_{kq} are used to predict the crystal-field parameters B_{kq} given by

$$B_{kq} = \rho_k A_{kq} \ , \qquad (1)$$

where the ρ_k are effective values of $\langle r^k \rangle$. The experimental data reported for Mn^{4+} in Cs_2GeF_6 are used to obtain an approximate set of ρ_k for the X^{4+} ions with the $3d^N$ electronic configuration. Because of the recent interest in the study of Cr^{4+} in a crystal-field of tetrahedral symmetry, we have calculated the energy levels of this ion in each of the host materials. In addition, we calculated the energy levels of all the X^{4+} ions with the $3d^N$ electronic configuration in the Ge site in $Bi_{12}GeO_{20}$. This latter calculation is done with and without the spin-orbit interaction.

2. Theory

The free ion Hamiltonian for a configuration of d^N ion is taken as

$$H_{FI} = F^{(2)}g_2 + F^{(4)}g_4 + \zeta \sum_{i=1}^{N} \vec{l}_i \cdot \vec{s}_i \ , \tag{2}$$

with

$$g_k = \sum_{i>j} \sum_{q=-k}^{k} C^*_{kq}(i)\, C_{kq}(j) \ , \tag{3}$$

and

$$C_{kq} = \sqrt{4\pi/(2k+1)}\, Y_{kq} \ . \tag{4}$$

The $F^{(k)}$ and ζ have been calculated with the use of Hartree-Fock wavefunctions [2], and determined by fitting the free-ion spectrum [3] and fitting the spectrum in solids [4]. The matrix elements of g_k, for all the states of the d^N configurations, are listed by Nielson and Koster [5], and we use their labels here. Frequently, the Racah parameters B and C are used in place of the Slater parameters, $F^{(k)}$, and the relations

$$F^{(2)} = 7(7B + C)$$

and

$$F^{(4)} = \frac{63}{5} C \tag{5}$$

can be used to convert from one set of parameters to the other. In general the Slater parameters are considerably reduced when an ion enters a solid. Furthermore, the values for these same parameters obtained by fitting the free ion spectra are less than the corresponding values computed by using Hartree-Fock wavefunctions. As an example of the reduction of the free-ion parameters, we have chosen Mn^{4+} in the host Cs_2GeF_6 with the parameters for each approximation listed in table 1 (from Morrison [4], p 133).

Table 1. Parameters for Mn^{4+} from Hartree-Fock, free-ion, and Cs_2GeF_6:Mn^{4+}

Parameters	Calculated[a] H–F	Experimental[b] free ion	Experimental[c] Cs_2GeF_6:Mn^{4+}
$F^{(2)}$ (cm^{-1})	101,615	86,939	55,644
$F^{(4)}$ (cm^{-1})	64,078	54,219	49,692
ζ (cm^{-1})	436	405	380
$\langle r^2 \rangle$ ($Å^2$)	0.3568	—	0.8104
$\langle r^4 \rangle$ ($Å^4$)	0.4097	—	2.114
B (cm^{-1})	1,347	1,160	572.2
C (cm^{-1})	5,086	4,303	3,944

[a]*Morrison [4], p 21;* [b]*p 14; and* [c]*p 133.*

We see that the reduction of B in going from the Hartree-Fock value to the value obtained for Mn^{4+} in Cs_2GeF_6 is quite large.

Further, the value Dq for Mn^{4+} in Cs_2GeF_6 is 2,185 cm^{-1} so that Dq/B = 3.82. Whereas, if the Dq is computed using $\langle r^4 \rangle$ from Hartree-Fock values, the crystal-field components, A_{40}, and equation (1), we have Dq = 368.5 cm^{-1} and Dq/B = 0.274, which is less than 1/10 the experimental value of Dq/B. Thus, values of Dq/B (which is one of the fundamental quantities extracted from comparing experiment when one uses a standard Tanabe-Sugano plot), calculated by Hartree-Fock values greatly underestimate the experimental values. This is not too surprising since the value of B decreases significantly when the ion enters the solid, whereas the radial wavefunction of the transition metal ion expands, causing an increase of $\langle r^4 \rangle$. These two effects cause the ratio Dq/B to increase dramatically.

From the values given in table 1 we find for Mn^{4+} in Cs_2GeF_6 that $F^{(2)}/F^{(2)}_{H-F}$ = 0.5476, $F^{(4)}/F^{(4)}_{H-F}$ = 0.7755, $\langle r^2 \rangle/\langle r^2 \rangle_{H-F}$ = 2.271, and $\langle r^4 \rangle/\langle r^4 \rangle_{H-F}$ = 5.159. We then assumed for the quadruply ionized $3d^N$ ions that $F^{(2)}$ = 0.5476 $F^{(2)}_{H-F}$, $F^{(4)}$ = 0.7755 $F^{(4)}_{H-F}$, ρ_2 = 2.271 $\langle r^2 \rangle_{H-F}$, and ρ_4 = 5.159 $\langle r^4 \rangle_{H-F}$. These values, along with the free-ion value of ζ, are given in table 2.

The crystal-field Hamiltonian for the electronic configuration d^N appropriate for the hosts here is

$$H_{CEF} = B_{20} \sum_{i=1}^{N} C_{20}(i) + B_{40} \sum_{i=1}^{N} C_{40}(i) + B_{44} \sum_{i=1}^{N} \left[C_{44}(i) + C_{4-4}(i) \right] \qquad (6)$$

with all B_{kq} real. In the cubic approximation, B_{20} = 0 and $B_{44} = (5/14)^{1/2} B_{40}$. If $B_{40} < 0$ then we have tetrahedral cubic symmetry and if $B_{40} > 0$ then the symmetry is octahedral. For both cases, B_{40} = 21 Dq. A large variety of different parameters are in use for the description of the crystal-field interaction of equation (6); for example, see Konig and Kremer [6]. The two most frequently quoted are from Ballhausen [7]:

$$B_{20} = -7Ds \ ,$$

$$B_{40} = -21\,Dq - 21\,Dt \ , \tag{7}$$

$$B_{44} = \frac{3}{2}\sqrt{70}\,Dq \ ,$$

and from Griffith [8]:

$$B_{20} = \delta - \mu \ ,$$

$$B_{40} = 21\,Dq - \left(\delta + \frac{3\mu}{4}\right)\sqrt{\frac{7}{10}} \ , \tag{8}$$

$$B_{44} = 3\sqrt{\frac{7}{10}}\,Dq + \left(\delta + \frac{3\mu}{4}\right)\sqrt{\frac{7}{10}} \ .$$

3. Parameters for Cr^{4+} and Cubic Approximation

The parameters ρ_2 and ρ_4 given in table 2 are used to obtain a set of crystal-field parameters, B_{kq}, for Cr^{4+} in each of the hosts. In obtaining the cubic approximate values, we use the rotational invariant, $S_k(X)$, defined as

$$S_k(X) = \left[\sum_{q=-k}^{k} X_{kq}^{*} X_{kq}\right]^{1/2} \ , \tag{9}$$

where X_{kq} is a spherical tensor such as the crystal-field components, A_{kq}, or crystal-field parameters, B_{kq}. Since for the cubic approximation to the crystal-field given in equation (6) we have $B_{40}^{c} = (5/14)^{1/2} B_{40}^{c}$, then

$$S_4^c(B) = \sqrt{\frac{12}{7}}\,B_{44}^c \tag{10}$$

with

$$S_4(A) = \sqrt{A_{40}^2 + 2A_{44}^2} \ , \tag{11}$$

and from equation (1) we have

$$B_{40}^c = \sqrt{\frac{7}{12}}\,\rho_4 S_4(A) \ , \tag{12}$$

and the sign of B_{40}^{c} is taken to be the same as A_{40}. The result given in equation (12) has been used with the monopole A_{kq} (see tables A-1.3, -1.4, -2.2, -3.3, and -3.4 in app A) to obtain the cubic approximation to the crystal-field parameters for Cr^{4+} in each of the host crystals. The

results are given in table 3 along with the Dq/B ratio for the cubic approximation ($B^c_{40} = 21\ Dq$). In the following text, the results of tables 2 and 3 will be used to calculate energy levels for Cr^{4+} in each of the host materials. Both the cubic approximation and the full symmetry of the site are considered. In these calculations we ignore the spin-orbit interaction since it is very small.

Since the Ge site in $Bi_{12}GeO_{20}$ has cubic symmetry, the A_{kq} from table A-4.4 (see app A) are used to construct the parameters given in table 4.

Table 2. Free-ion parameters (cm^{-1}) and effective ρ_k ($Å^k$) for quadruply ionized ionic of the $3d^N$ series derived from Cs_2GeF_6 experimental[a]

Ion	nd^N	$F^{(2)}$ B	$F^{(4)}$ C	ζ	ρ_2	ρ_4
V	$3d^1$	— —	— —	250	0.9988	3.350
Cr	$3d^2$	52,726 541.6	47,131 3,741	319	0.8421	2.168
Mn	$3d^3$	55,644 572.2	49,692 3,944	405	0.8103	2.114
Fe	$3d^4$	58,465 601.7	52,160 4,140	513	0.6618	1.386
Co	$3d^5$	61,393 632.3	54,736 4,344	654	0.6179	1.172
Ni	$3d^6$	63,611 656.2	56,620 4,494	830	0.5671	0.9673
Cu	$3d^7$	66,073 682.4	58,743 4,662	1,008	0.5185	0.7862
Zn	$3d^8$	68,582 709.1	60,914 4,834	1,203	0.4769	0.6191
Ga	$3d^9$	— —	— —	1,496	0.40878	0.4127

[a] *$F^{(2)} = 0.5476\ F^{(2)}_{H-F}$, $F^{(4)} = 0.7755\ F^{(4)}_{H-F}$, ζ = free-ion — except for Ga^{4+}; for Ga^{4+}, $\zeta = \zeta_{H-F}$ — $\rho_2 = 2.271\ \langle r^2\rangle_{H-F}$, and $\rho_4 = 5.159\ \langle r^4\rangle_{H-F}$. All the Hartree-Fock data and free-ion data are from Morrison [4], p 21.*

Table 3. Approximate crystal-field parameters (cm^{-1}) for Cr^{4+} in the four host materials

No.	Host	Symmetry	B_{40}[a]	Dq/B	B_{20}	B_{40}	B_{44}	Table No.
1	Na_2TiSiO_5[b]	C_{4v}	39,297	3.46	15,959	39,148	23,610	4.1 and 4.2
2	Na_2TiSiO_5[c]	D_{2d}	–65,526	5.76	6,135	–68,134	–36,856	4.3 and 4.4
3	Y_2SiBeO_7	S_4	–59,251	5.21	8,445	–62,421	–32,574	4.5 and 4.6
4	$Bi_4Si_3O_{12}$	S_4	–68,043	5.98	–3,724	–64,793	–43,236	4.7 and 4.8
5	$Bi_4Ge_3O_{12}$	S_4	–48,292	4.25	–7,704	–41,352	–33,429	4.9 and 4.10

[a]*Cubic approximation* $B_{44} = \sqrt{5/14}\ B_{40}$.
[b]*Ti site.*
[c]*Si site.*

Table 4. Approximate crystal-field parameters (cm^{-1}) for X^{4+} in the Ge site (T symmetry) in $Bi_{12}GeO_{20}$

Ion	$3d^N$	B_{40}[a]	Dq/B
V	$3d^1$	–84,923	—
Cr	$3d^2$	–54,959	4.83
Mn	$3d^3$	–53,590	4.46
Fe	$3d^4$	–35,135	2.78
Co	$3d^5$	–29,710	2.24
Ni	$3d^6$	–24,521	1.78
Cu	$3d^7$	–19,930	1.39
Zn	$3d^8$	–15,694	1.05
Ga	$3d^9$	–10,462	—

[a]$B_{44} = \sqrt{\frac{5}{14}}\ B_{40}$.

4. Energy Level of Cr^{4+} in Each Host

4.1 Cr^{4+}:Na_2TiSiO_5

4.1.1 Ti Site

The parameters to be used in equations (2) and (6) for the calculation of the energy levels of Cr^{4+} in the Ti site from tables 2 and 3 are $F^{(2)}$ = 52,726; $F^{(4)}$ = 47,131; and B^c_{40} = 39,297 (cm^{-1}), with $B^c_{44} = (5/14)^{1/2} B^c_{40}$. The results are given in table 5.1. With the same $F^{(k)}$, but with B_{20} = 15,959; B_{40} = 39,148; and B_{44} = 23,610 (cm^{-1}) (C_{4v} symmetry), the results are given in table 5.2. In the cubic symmetry (octahedral) the ground state is $^3T_1(F)$, which in the full C_{4v} symmetry splits into a Γ_5 (E = 0) and Γ_2 with a splitting of 6300 cm^{-1}. This large splitting is caused by the very large value of B_{20} since the ratio of B_{44}/B_{40} is very close to the cubic ratio $(5/14)^{1/2}$. The ^1E level is split (Γ_1 and Γ_3 in C_{4v}) by approximately 17,000 cm^{-1} so that the Γ_1 at 6,640 cm^{-1} and the Γ_3 at 17,899 cm^{-1} encompass the $^1T_2$ (Γ_4 and Γ_5 in C_{4v}). However, the largest splitting is the $^3T_1(P)$ at 24,467 cm^{-1} which in the C_{4v} symmetry forms a Γ_2 at 18,091 cm^{-1} and a Γ_5 at 32,363 cm^{-1} encompassing the $^3T_2$, which suffers a comparatively small splitting (~1050 cm^{-1}). These results indicate that it would be next to impossible to interpret the experimental data in terms of cubic symmetry, assuming that the approximate values of the parameters are reasonable.

4.1.2 Si Site

The parameter for the cubic approximation is B^c_{40} = –65,526 cm^{-1} and for the full D_{2d} symmetry, B_{20} = 6135; B_{40} = –68,134; and B_{44} = –36,856 (cm^{-1}). The cubic results are given in table 5.3, and the D_{2d} results are in table 5.4. The $^3A_2$ ground state in cubic symmetry goes over to the Γ_3 state. (In the presence of spin-orbit coupling with ζ = 319 cm^{-1}, this state becomes a Γ_5 doublet and a Γ_4 singlet with the Γ_5 lowest and the Γ_4 at 0.14 cm^{-1}.) The ^1E level in cubic symmetry is split into a Γ_1 and Γ_3 with a splitting of 369 cm^{-1}. The $^3T_2$ band is split into a Γ_5 and Γ_4 band, and the $^3T_1(P)$ is split into a Γ_2 and Γ_5 band. However, these splittings are not too severe and a first analysis could be done, assuming tetrahedral cubic symmetry.

4.2 Cr^{4+}:$Y_2SiBe_2O_7$

The free-ion parameters given in table 2 and the crystal-field parameters given in table 3 are used to calculate the energy levels of Cr^{4+} in this host. The calculation for the cubic approximation is given in table 5.5; and for S_4 symmetry, in table 5.6. The $^3A_2$ level in the cubic approximation remains the lowest level in S_4 symmetry despite the

rather large value of B_{20}. However, the ^1E level is split by 795 cm^{-1} which might lead to an experimental error in identification using cubic symmetry. Further, the $^3T_2$ is split by approximately 3000 cm^{-1} and the $^3T_1(P)$ is split by approximately 7500 cm^{-1}, both of which could lead to confusion if the experimental data are interpreted in terms of a cubic approximation. The experimental data might be analyzed in cubic symmetry provided the above deviations are considered.

4.3 Cr^{4+}:$Bi_4X_3O_{12}$ (X = Ge, Si)

4.3.1 $Bi_4Si_3O_{12}$

With the use of the parameters of tables 2 and 3, the energy levels of Cr^{4+} in the Si site in this host were calculated, with the results given in tables 5.7 (cubic approximation) and 5.8 (S_4 symmetry). The splitting of the cubic ^1E level by the S_4 symmetry crystal field is only 6 cm^{-1}, the splitting of the $^3T_2$ is approximately 3000 cm^{-1}, and that of the $^3T_1(P)$ is 3500 cm^{-1}. The experimental data on Cr^{4+} in this host can be crudely analyzed assuming a cubic approximation if one is aware of the possible large splitting of the $^3T_2$ and $^3T_1(P)$ states.

4.3.2 $Bi_4Ge_3O_{12}$

The parameters given in tables 2 and 3 are used to calculate the splittings of the levels of Cr^{4+} in this host. The results are given in tables 5.9 and 5.10. The splittings in the cubic approximation are smaller than in the previous host. However, the large value of B_{20} causes a greater splitting of the ^1E (66 cm^{-1}). Also, the large value of B_{20} causes the $^3T_1(F)$ to intersperse with the $^3T_1(P)$. This mixture of the cubic terms would make the analysis of the experimental data on Cr^{4+} in terms of a cubic approximation next to impossible.

Table 5. Energy levels (cm^{-1}) of Cr^{4+} using the parameters of tables 2 and 3:
5.1 For Ti site in Na_2TiSiO, cubic approximation, no spin-orbit

Level	I.R.[a]	Energy (cm^{-1})	Free ion state
1	$^3T_1$ (F)	0	0.90 ^3F + 0.10 ^3P
2	$^1T_2$	10,979	0.53 ^1D + 0.47 ^1G
3	^1E	11,075	0.52 ^1G + 0.48 ^1D
4	$^3T_2$	17,527	1.00 ^3F
5	$^1A_1$	23,435	0.71 ^1G + 0.29 ^1S
6	$^3T_1$ (P)	24,467	0.90 ^3P + 0.10 ^3F
7	$^1T_2$	29,533	0.53 ^1G + 0.47 ^1D
8	$^1T_1$	31,508	1.00 ^1G
9	$^3A_2$	36,240	1.00 ^3F
10	^1E	48,150	0.52 ^1D + 0.48 ^1G
11	$^1A_1$	63,701	0.71 ^1S + 0.29 ^1G

[a]*Irreducible representation of the O or T_d group, Mulligan notation.*

5.2 For Ti site in Na_2TiSiO_5, C_{4v} symmetry, no spin-orbit

Level	I.R.[a]	Energy (cm^{-1})	Free ion state
1	Γ_5	0	0.88 ^3F + 0.12 ^3P
2	Γ_2	6,299	0.97 ^3F + 0.03 ^3P
3	Γ_1	6,639	0.55 ^1G + 0.41 ^1D + 0.04 ^1S
4	Γ_5	10,907	0.52 ^1D + 0.48 ^1G
5	Γ_4	17,751	0.56 ^1D + 0.44 ^1G
6	Γ_3	17,899	0.51 ^1G + 0.49 ^1D
7	Γ_2	18,091	0.97 ^3P + 0.03 ^3F
8	Γ_5	18,601	0.92 ^3F + 0.08 ^3P
9	Γ_4	19,648	1.00 ^3F
10	Γ_2	24,595	1.00 ^1G
11	Γ_1	27,151	0.68 ^1G + 0.22 ^1S + 0.10 ^1D
12	Γ_5	29,962	0.61 ^1G + 0.39 ^1D
13	Γ_4	31,719	0.56 ^1G + 0.44 ^1D
14	Γ_5	32,362	0.80 ^3P + 0.20 ^3F
15	Γ_3	38,461	1.00 ^3F
16	Γ_5	40,120	0.91 ^1G + 0.09 ^1D
17	Γ_1	47,074	0.44 ^1G + 0.39 ^1D + 0.17 ^1S
18	Γ_3	50,384	0.51 ^1D + 0.49 ^1G
19	Γ_1	69,763	0.57 ^1S + 0.33 ^1G + 0.10 ^1D

[a]*Irreducible representation of the C_{4v} group (Bethe notation, G. F. Koster, J. O. Dimmock, R. G. Wheeler, and H. Statz, Properties of the thirty-two point groups, MIT Press, Cambridge, MA (1963)).*

C_{4v} group selection rules for electric dipole transitions

A. Single group

I.R.	Γ_1	Γ_2	Γ_3	Γ_4	Γ_5
Γ_1	π	0	0	0	σ
Γ_2	0	π	0	0	σ
Γ_3	0	0	π	0	σ
Γ_4	0	0	0	π	σ
Γ_5	σ	σ	σ	σ	π

B. Double group

I.R.	Γ_6	Γ_7
Γ_6	π,σ	σ
Γ_7	σ	π,σ

Table 5. Energy levels (cm^{-1}) of Cr^{4+} using the parameters of tables 2 and 3 (cont'd):
5.3 For Si site in Na_2TiSiO_5, cubic approximation, no spin-orbit

Level	I.R.[a]	Energy	Free ion state
1	$^3A_2$	0	1.00 ^3F
2	^1E	11,758	0.60 ^1D + 0.40 ^1G
3	$^1A_1$	21,612	0.76 ^1G + 0.24 ^1S
4	$^3T_2$	31,202	1.00 ^3F
5	$^3T_1$	37,307	0.70 ^3P + 0.30 ^3F
6	$^1T_2$	42,906	0.63 ^1D + 0.37 ^1G
7	$^1T_1$	45,184	1.00 ^1G
8	$^3T_1$	64,426	0.70 ^3F + 0.30 ^3P
9	^1E	74,817	0.60 ^1G + 0.40 ^1D
10	$^1T_2$	74,872	0.63 ^1G + 0.37 ^1D
11	$^1A_1$	92,874	0.76 ^1S + 0.24 ^1G

[a]*Irreducible representation of the O or T_d group (Mulligan notation).*

5.4 For Si site in Na_2TiSiO_5, D_{2d} symmetry, no spin-orbit

Level	I.R.[a]	Energy	Free ion state
1	Γ_3	0	1.00 ^3F
2	Γ_1	11,392	0.58 ^1D + 0.41 ^1G + 0.01 ^1S
3	Γ_3	11,760	0.60 ^1D + 0.40 ^1G
4	Γ_1	21,961	0.74 ^1G + 0.23 ^1S + 0.02 ^1D
5	Γ_4	29,374	1.00 ^3F
6	Γ_5	31,960	0.99 ^3F + 0.01 ^3P
7	Γ_2	33,585	0.72 ^3P + 0.28 ^3F
8	Γ_5	39,196	0.67 ^3P + 0.33 ^3F
9	Γ_4	41,092	0.62 ^1D + 0.38 ^1G
10	Γ_2	41,385	1.00 ^1G
11	Γ_5	43,547	0.60 ^1D + 0.40 ^1G
12	Γ_5	47,235	0.96 ^1G + 0.04 ^1D
13	Γ_5	63,018	0.68 ^3F + 0.32 ^3P
14	Γ_2	67,051	0.72 ^3F + 0.28 ^3P
15	Γ_1	71,288	0.59 ^1G + 0.38 ^1D + 0.03 ^1S
16	Γ_5	73,418	0.63 ^1G + 0.37 ^1D
17	Γ_3	77,517	0.60 ^1G + 0.40 ^1D
18	Γ_4	77,560	0.62 ^1G + 0.38 ^1D
19	Γ_1	93,496	0.73 ^1S + 0.25 ^1G + 0.01 ^1D

[a]*Irreducible representations of the D_{2d} group (G. F. Koster, J. O. Dimmock, R. G. Wheeler, and H. Statz, Properties of the thirty-two point groups, MIT Press, Cambridge, MA (1963)).*

D_{2d} group selection rules for electric dipole transitions

A. Single group

I.R.	Γ_1	Γ_2	Γ_3	Γ_4	Γ_5
Γ_1	0	0	0	π	σ
Γ_2	0	0	π	0	σ
Γ_3	0	π	0	0	σ
Γ_4	π	0	0	0	σ
Γ_5	σ	σ	σ	σ	π

B. Double group

I.R.	Γ_6	Γ_7
Γ_6	σ	π,σ
Γ_7	π,σ	σ

Table 5. Energy levels (cm^{-1}) of Cr^{4+} using the parameters of tables 2 and 3 (cont'd):
5.5 For Si site in $Y_2SiBe_2O_7$, cubic approximation, no spin orbit

No.	I.R.[a]	Energy (cm^{-1})	Free ion state
1	$^3A_2$	0	1.00 ^3F
2	^1E	11,752	0.60 ^1D + 0.40 ^1G
3	$^1A_1$	21,428	0.77 ^1G + 0.23 ^1S
4	$^3T_2$	28,214	1.00 ^3F
5	$^3T_1$ (*P*)	34,270	0.68 ^3P + 0.32 ^3F
6	$^1T_2$	39,907	0.63 ^1D + 0.37 ^1G
7	$^1T_1$	42,195	1.00 ^1G
8	$^3T_1$ (*F*)	58,498	0.68 ^3F + 0.32 ^3P
9	^1E	68,847	0.60 ^1G + 0.40 ^1D
10	$^1T_2$	68,907	0.63 ^1G + 0.37 ^1D
11	$^1A_1$	87,082	0.77 ^1S + 0.23 ^1G

[a]*Irreducible representations of the T_d or O group (Mulligan notation).*

5.6 For Si site in $Y_2SiBe_2O_7$, S_4 symmetry, no spin-orbit

No.	I.R.[a]	Energy (cm^{-1})	Free ion state
1	Γ_2	0	1.00 ^3F
2	Γ_1	10,960	0.56 ^1D + 0.42 ^1G + 0.02 ^1S
3	Γ_2	11,756	0.60 ^1D + 0.40 ^1G
4	Γ_1	22,179	0.74 ^1G + 0.21 ^1S + 0.05 ^1D
5	Γ_2	25,955	1.00 ^3F
6	$\Gamma_{3,4}$	29,044	0.98 ^3F + 0.02 ^3P
7	Γ_1	29,188	0.71 ^3P + 0.29 ^3F
8	$\Gamma_{3,4}$	36,886	0.63 ^3P + 0.37 ^3F
9	Γ_1	36,995	1.00 ^1G
10	Γ_2	37,668	0.62 ^1D + 0.38 ^1G
11	$\Gamma_{3,4}$	40,543	0.59 ^1D + 0.41 ^1G
12	$\Gamma_{3,4}$	45,092	0.94 ^1G + 0.06 ^1D
13	$\Gamma_{3,4}$	56,644	0.65 ^3F + 0.35 ^3P
14	Γ_1	61,927	0.71 ^3F + 0.29 ^3P
15	Γ_1	63,966	0.59 ^1G + 0.37 ^1D + 0.04 ^1S
16	$\Gamma_{3,4}$	66,965	0.64 ^1G + 0.36 ^1D
17	Γ_2	72,391	0.60 ^1G + 0.40 ^1D
18	Γ_2	72,434	0.62 ^1G + 0.38 ^1D
19	Γ_1	88,092	0.73 ^1S + 0.25 ^1G + 0.02 ^1D

[a]*Irreducible representations of the S_4 group, $\Gamma_{3,4} = \Gamma_3 + \Gamma_4$ (Bethe notation, G. F. Koster, J. O. Dimmock, R. G. Wheeler, and H. Statz, Properties of the thirty-two point groups, MIT Press, Cambridge, MA (1963)).*

S_4 group selection rules for electric dipole transitions

A. Single group

I.R.	Γ_1	Γ_2	Γ_3	Γ_4
Γ_1	0	π	σ	σ
Γ_2	π	0	σ	σ
Γ_3	σ	σ	0	π
Γ_4	σ	σ	π	0

B. Double group

I.R.	Γ_5	Γ_6	Γ_7	Γ_8
Γ_5	0	σ	π	σ
Γ_6	σ	0	σ	π
Γ_7	π	σ	0	σ
Γ_8	σ	π	σ	0

Table 5. Energy levels (cm^{-1}) of Cr^{4+} using the parameters of tables 2 and 3 (cont'd):
5.7 For Si site in $Bi_4Si_3O_{12}$, cubic approximation, no spin-orbit

No.	I.R.[a]	Energy (cm^{-1})	Free ion state
1	$^3A_2$	0	1.00 ^3F
2	^1E	11,760	0.60 ^1D + 0.40 ^1G
3	$^1A_1$	21,678	0.75 ^1G + 0.25 ^1S
4	$^3T_2$	32,401	1.00 ^3F
5	$^3T_1$ (P)	38,523	0.70 ^3P + 0.30 ^3F
6	$^1T_2$	44,109	0.63 ^1D + 0.37 ^1G
7	$^1T_1$	46,382	1.00 ^1G
8	$^3T_1$ (F)	66,806	0.70 ^3F + 0.30 ^3P
9	^1E	77,212	0.60 ^1G + 0.40 ^1D
10	$^1T_2$	77,265	0.63 ^1G + 0.37 ^1D
11	$^1A_1$	95,206	0.75 ^1S + 0.25 ^1G

[a]*Irreducible representations of the T_d or O group (Mulligan notation).*

5.8 For Si site in $Bi_4Si_3O_{12}$, S_4 symmetry, no spin-orbit

No.	I.R.[a]	Energy (cm^{-1})	Free ion state
1	Γ_2	0	1.00 ^3F
2	Γ_1	11,752	0.60 ^1D + 0.40 ^1G
3	Γ_2	11,759	0.60 ^1D + 0.40 ^1G
4	Γ_1	21,680	0.75 ^1G + 0.25 ^1S
5	$\Gamma_{3,4}$	31,300	1.00 ^3F
6	Γ_2	34,451	1.00 ^3F
7	$\Gamma_{3,4}$	37,292	0.71 ^3P + 0.29 ^3F
8	Γ_1	40,826	0.68 ^3P + 0.32 ^3F
9	$\Gamma_{3,4}$	43,008	0.62 ^1D + 0.38 ^1G
10	$\Gamma_{3,4}$	45,129	1.00 ^1G
11	Γ_2	46,142	0.64 ^1D + 0.36 ^1G
12	Γ_1	48,761	1.00 ^1G
13	Γ_1	64,521	0.68 ^3F + 0.32 ^3P
14	$\Gamma_{3,4}$	67,812	0.71 ^3F + 0.29 ^3P
15	Γ_2	74,854	0.60 ^1G + 0.40 ^1D
16	Γ_2	74,921	0.64 ^1G + 0.36 ^1D
17	$\Gamma_{3,4}$	78,293	0.62 ^1G + 0.38 ^1D
18	Γ_1	78,772	0.59 ^1G + 0.39 ^1D + 0.03 ^1S
19	Γ_1	95,721	0.72 ^1S + 0.26 ^1G + 0.01 ^1D

[a]*Irreducible representations of the S_4 group, $\Gamma_{3,4} = \Gamma_3 + \Gamma_4$ (Bethe notation, G. F. Koster, J. O. Dimmock, R. G. Wheeler, and H. Statz, Properties of the thirty-two point groups, MIT Press, Cambridge, MA (1963)).*

Note: See table 5.6 for allowed transitions.

Table 5. Energy levels (cm^{-1}) of Cr^{4+} using the parameters of tables 2 and 3 (cont'd):
5.9 For Ge site in $Bi_4Ge_3O_{12}$, cubic approximation, no spin-orbit

No.	I.R.[a]	Energy (cm^{-1})	Free ion state
1	$^3A_2$	0	1.00 ^3F
2	^1E	11,738	0.61 ^1D + 0.39 ^1G
3	$^1A_1$	21,015	0.80 ^1G + 0.20 ^1S
4	$^3T_2$	22,996	1.00 ^3F
5	$^3T_1(P)$	28,931	0.65 ^3P + 0.35 ^3F
6	$^1T_2$	34,662	0.65 ^1D + 0.35 ^1G
7	$^1T_1$	36,977	1.00 ^1G
8	$^3T_1(F)$	48,182	0.65 ^3F + 0.35 ^3P
9	^1E	58,424	0.61 ^1G + 0.39 ^1D
10	$^1T_2$	58,497	0.65 ^1G + 0.35 ^1D
11	$^1A_1$	77,058	0.80 ^1S + 0.20 ^1G

[a]*Irreducible representations of the T_d or O group (Mulligan notation).*

5.10 For Ge site in $Bi_4Ge_3O_{12}$, S_4 symmetry, no spin-orbit

No.	I.R.[a]	Energy (cm^{-1})	Free ion state
1	Γ_2	0	1.00 ^3F
2	Γ_1	11,663	0.60 ^1D + 0.40 ^1G
3	$\Gamma_{3,4}$	11,729	0.62 ^1D + 0.38 ^1G
4	$\Gamma_{3,4}$	20,531	1.00 ^3F
5	Γ_1	21,004	0.80 ^1G + 0.19 ^1S + 0.01 ^1D
6	$\Gamma_{3,4}$	26,162	0.67 ^3P + 0.33 ^3F
7	Γ_2	26,636	1.00 ^3F
8	$\Gamma_{3,4}$	32,162	0.61 ^1D + 0.39 ^1G
9	Γ_1	32,936	0.51 ^3F + 0.49 ^3P
10	$\Gamma_{3,4}$	34,160	0.97 ^1G + 0.03 ^1D
11	Γ_2	38,213	0.69 ^1D + 0.31 ^1G
12	Γ_1	41,547	1.00 ^1G
13	Γ_1	43,409	0.51 ^3P + 0.49 ^3F
14	$\Gamma_{3,4}$	49,514	0.68 ^3F + 0.32 ^3P
15	Γ_2	53,095	0.62 ^1G + 0.38 ^1D
16	Γ_2	53,248	0.69 ^1G + 0.31 ^1D
17	Γ_1	59,816	0.55 ^1G + 0.34 ^1D + 0.11 ^1S
18	$\Gamma_{3,4}$	59,912	0.64 ^1G + 0.36 ^1D
19	Γ_1	78,626	0.69 ^1S + 0.26 ^1G + 0.05 ^1D

[a]*Irreducible representations of the S_4 group, $\Gamma_{3,4} = \Gamma_3 + \Gamma_4$ (Bethe notation, G. F. Koster, J. O. Dimmock, R. G. Wheeler, and H. Statz, Properties of the thirty-two point groups, MIT Press, Cambridge, MA (1963)).*

Note: See table 5.6 for allowed transitions.

5. Energy Levels of the X^{4+} Ions in $Bi_{12}GeO_{20}$

Because of the technological importance of the compounds $Bi_{12}XO_{20}$ (X = Ge, Si) [9,10], we have decided to calculate the energy levels of the entire $3d^N$ series of X^{4+} ions assuming these ions replace the Ge site substitutionally. Also, the Ge (Si) site in these compounds has the unique distinction of being of the cubic group T, and the optical spectra of these ions should be quite interesting. The parameters used in the calculations are given in tables 2 and 4, and the results are given in tables 6 to 23. For each ion, the energy levels are calculated with the spin-orbit interaction "turned off," followed by a similar calculation with the spin-orbit parameter values given in table 2. The optical spectra of Cr^{4+} in $Bi_{12}GeO_{20}$ have been reported by Wardzynski et al [11], who give B_{40} = –17,220 cm^{-1} and B = 428.8 cm^{-1}, giving the parameter Dq/B = 1.91, whereas our estimated value, Dq/B = 4.83, is much larger. This would indicate that our estimate of Dq is too large or B is too small. However, their reported energy levels correspond more closely to the levels of Fe^{4+} (tables 12 and 13) calculated here.

The labeling of the levels is the irreducible representation of the T groups in the Bethe notation [12]. The correspondence with the T_d group in Mulligan notation is as follows: A_1 and A_2 correspond to Γ_1, E becomes $\Gamma_2 + \Gamma_3$ (still a doublet), and T_1 and T_2 correspond to the triplet Γ_4. The double group Γ_6 and Γ_7 (T_d) corresponds to Γ_5 (T), and the quartet Γ_8 (T_d) becomes $\Gamma_6 + \Gamma_7$ (T), which is two degenerate doublets. For d electrons the difference between the T and T_d groups is insignificant, but for f electrons there is a distinct difference. In the absence of the spin-orbit interaction, the energy levels can be obtained from a Tanabe-Sugano plot for ions with the d^N configurations provided the complementary rules are observed for tetrahedral symmetry. That is, for the configuration d^N in tetrahedral symmetry, we use the d^{10-N} Tanabe-Sugano plot. (These standard plots are for octahedral symmetry.) The inclusion of the spin-orbit interaction has very little effect on the V^{4+}, Cr^{4+}, and Mn^{4+} ions. However, in the Fe^{4+} ion (table 13) the Γ_1 ground state in the absence of spin-orbit (40 percent ^1I) remains Γ_1 but is 67 percent ^5D with 11 percent ^1I. This mixture could be changed considerably by different values of Dq/B. The spin-orbit interaction causes the ^6S ground state of Co^{4+} with $\zeta = 0$ to split into a Γ_5 level at $E = 0$ and a four-fold degenerate level $\Gamma_{6,7}$ to split at 0.04 cm^{-1} (table 15).

For the ion Ni^{4+} the $\Gamma_{2,3}$ level of the ground state with $\zeta = 0$ is split into 5 levels ($0 \leq E \leq 176$ cm^{-1}) by the spin-orbit interaction, as shown in tables 16 and 17. Also the spin-orbit mixes different spin states beginning with the Γ_4 levels at 11,142 cm^{-1}. The Cu^{4+} ion energy levels given in table 19 show that the first excited state is mixed by the spin-orbit interaction (98 percent ^4F + 1 percent ^2G) with the higher energy

levels becoming strongly mixed. Similarly, for the energy levels of Zn^{4+}, table 21, and Ga^{4+}, table 23, the spin-orbit interaction has a reasonably strong effect on the composition of the wave functions for the higher energy levels. This mixture of different total spin raises the spin forbidden transition rules usually employed in the interpretation of $3d^N$ electronic configuration optical absorption data.

The only ion with experimental data other than Cr^{4+} that we were able to find was Fe^{4+} [13], and we have not investigated this ionization state here.

The interstitial site mentioned [14] for $Bi_{12}GeO_{20}$ was investigated. The statement concerning the size of this site (6b in the crystallographic data) is correct. In the host material $Bi_{12}GeO_{20}$, the nearest neighbors at this site have four Bi ions at 2.86 Å while the Bi site has eight oxygen ions ranging from 2.08 to 3.47 Å and the Ge ion has four oxygen ions at 1.72 Å. However, because the nearest neighbors are Bi^{3+} it seems that it would be difficult to trap a positive ion at this position. On the other hand, this site might act as an electron trapping center in this crystal (also the silicon counterpart). Nevertheless, the monopole crystal-field components, A_{kq} ($cm^{-1}/Å^k$), were calculated, with $A_{20} = -31{,}713$; $A_{22} = 19{,}514$; $A_{40} = 4{,}521$; $A_{42} = 7{,}866$; and $A_{44} = -613$, and the site has D_2 symmetry. If this site had D_{2d} symmetry then A_{22} and A_{42} would vanish, which appears to be rather a gross assumption considering the relative magnitude of these components.

A second possible interstitial site not mentioned by Wardzynski and Szymczak [14] is the site (12d) which is located at (0, 0, 1/4) and has C_2 symmetry. This site has for nearest neighbors two Bi ions at 1.92 Å, two O ions at 2.09 Å, and one Ge ion at 2.54 Å. The monopole crystal-field components A_{kq} ($cm^{-1}/Å^k$) are as follows: $A_{20} = 12{,}856$; $A_{22} = 47{,}509 + i15{,}341$; $A_{40} = -7{,}415$; $A_{42} = -111 + i6{,}203$; and $A_{44} = -11{,}806 - i3{,}334$. The two-fold fields are slightly larger (absolute magnitude) than the previous interstitial site but this site has, in addition, a large A_{10} component (48,637 $cm^{-1}/Å$) which is equivalent to a constant electric field in the z direction. In view of these factors, this site does not appear to be a possible electron trapping site for electrons, but further work would be necessary to determine if a doubly ionized transition-metal ion might occupy it.

Table 6. Energy levels (cm^{-1}) for V^{4+} using the parameters of tables 2 and 4, for Ge site in $Bi_{12}GeO_{20}$, T symmetry, no spin orbit

No.	I.R.[a]	Energy (cm^{-1})	Free ion state
1	$\Gamma_{2,3}$	0	1.00 ^2D
2	Γ_4	40,439	1.00 ^2D

[a]*Irreducible representations of the T group, $\Gamma_{2,3} = \Gamma_2 + \Gamma_3$ (Bethe notation, G. F. Koster, J. O. Dimmock, R. G. Wheeler, and H. Statz, Properties of the thirty-two point groups, MIT Press, Cambridge, MA (1963)).*

Table 7. Energy levels (cm^{-1}) for V^{4+} using the parameters of tables 2 and 4, for Ge site in $Bi_{12}GeO_{20}$, T symmetry, $\zeta = 250\ cm^{-1}$

No.	I.R.[a]	Energy (cm^{-1})	Free ion state
1	$\Gamma_{6,7}$	0	1.00 ^2D
2	$\Gamma_{6,7}$	40,319	1.00 ^2D
3	Γ_5	40,691	1.00 ^2D

[a]*Irreducible representations of the double T (cubic) group (G. F. Koster, J. O. Dimmock, R. G. Wheeler, and H. Statz, Properties of the thirty-two point groups, MIT Press, Cambridge, MA (1963)).*

Table 8. Energy levels (cm^{-1}) for Cr^{4+} using the parameters of tables 2 and 4, for Ge site in $Bi_{12}GeO_{20}$, T symmetry, no spin orbit

No.	I.R.[a]	Energy (cm^{-1})	Free ion state
1	Γ_1	0	1.00 ^3F
2	$\Gamma_{2,3}$	11,748	0.61 ^1D + 0.39 ^1G
3	Γ_1	21,282	0.78 ^1G + 0.22 1S
4	Γ_4	26,170	1.00 ^3F
5	Γ_4	32,186	0.67 ^3P + 0.33 ^3F
6	Γ_4	37,854	0.64 ^1D + 0.36 ^1G
7	Γ_4	40,152	1.00 ^1G
8	Γ_4	54,451	0.67 ^3F + 0.33 ^3P
9	$\Gamma_{2,3}$	64,764	0.61 ^1G + 0.39 ^1D
10	Γ_4	64,829	0.64 ^1G + 0.36 ^1D
11	Γ_1	83,140	0.78 ^1S + 0.22 ^1G

[a]*Irreducible representations of the T (cubic) group, $\Gamma_{2,3} = \Gamma_2 + \Gamma_3$ (Bethe notation, G. F. Koster, J. O. Dimmock, R. G. Wheeler, and H. Statz, Properties of the thirty-two point groups, MIT Press, Cambridge, MA (1963)).*

Table 9. Energy levels (cm^{-1}) for Cr^{4+} using the parameters of tables 2 and 4, for Ge site in $Bi_{12}GeO_{20}$, T symmetry, $\zeta = 319\ cm^{-1}$

No.	I.R.[a]	Energy (cm^{-1})	Free ion state		
1	Γ_4	0	1.00 ^3F		
2	$\Gamma_{2,3}$	11,739	0.61 ^1D	+	0.39 ^1S
3	Γ_1	21,273	0.78 ^1G	+	0.22 ^1S
4	Γ_1	26,021	1.00 ^3F		
5	Γ_4	26,096	1.00 ^3F		
6	$\Gamma_{2,3}$	26,249	1.00 ^3F		
7	Γ_4	26,251	1.00 ^3F		
8	Γ_1	32,149	0.68 ^3P	+	0.31 ^3F
9	Γ_4	32,169	0.68 ^3P	+	0.32 ^3F
10	Γ_4	32,223	0.66 ^3P	+	0.34 ^3F
11	$\Gamma_{2,3}$	32,239	0.66 ^3P	+	0.34 ^3F
12	Γ_4	37,861	0.64 ^1D	+	0.36 ^1S
13	Γ_4	40,164	1.00 ^1G		
14	$\Gamma_{2,3}$	54,360	0.66 ^3F	+	0.34 ^3P
15	Γ_4	54,365	0.66 ^3F	+	0.34 ^3P
16	Γ_4	54,577	0.68 ^3F	+	0.32 ^3P
17	Γ_1	54,674	0.69 ^3F	+	0.31 ^3P
18	$\Gamma_{2,3}$	64,784	0.61 ^1G	+	0.39 ^1D
19	Γ_4	64,849	0.64 ^1G	+	0.36 ^1D
20	Γ_1	83,165	0.78 ^1S	+	0.22 ^1S

[a]Irreducible representations of the T group, $\Gamma_{2,3} = \Gamma_2 + \Gamma_3$ (degenerate doublets) (G. F. Koster, J. O. Dimmock, R. G. Wheeler, and H. Statz, Properties of the thirty-two point groups, MIT Press, Cambridge, MA (1963)).

Table 10. Energy levels (cm^{-1}) for Mn^{4+} using the parameters of tables 2 and 4, for Ge site in $Bi_{12}GeO_{20}$, T symmetry, no spin orbit

No.	I.R.[a]	Energy (cm^{-1})	Free ion state
1	$\Gamma_{2,3}$	0	0.40 ^2G + 0.32 ^2H + 0.15 $^2D1$
2	Γ_4	8,233	0.88 ^4F + 0.12 ^4P
3	Γ_4	22,675	0.56 ^2H + 0.44 ^2G
4	Γ_4	23,652	0.51 ^2G + 0.24 $^2D2$ + 0.16 ^2H
5	Γ_4	26,721	0.54 ^2P + 0.27 ^2F + 0.19 ^2H
6	Γ_4	32,415	1.00 ^4F
7	Γ_4	37,865	0.37 ^2H + 0.29 ^2F + 0.24 $^2D1$
8	Γ_4	39,661	0.88 ^4P + 0.12 ^4F
9	Γ_1	46,535	1.00 ^2G
10	Γ_4	48,689	0.60 ^2H + 0.25 ^2G + 0.14 ^2P
11	Γ_4	49,882	0.43 ^2G + 0.30 $^2D2$ + 0.15 ^2H
12	$\Gamma_{2,3}$	50,480	0.50 ^2H + 0.43 $^2D2$ + 0.06 $^2D1$
13	Γ_4	53,810	0.55 ^2F + 0.35 ^2H + 0.06 ^2G
14	Γ_4	54,639	0.40 $^2D2$ + 0.40 ^2F + 0.18 ^2H
15	Γ_1	57,979	1.00 ^2F
16	Γ_1	57,980	1.00 ^2F
17	$\Gamma_{2,3}$	68,057	0.51 $^2D1$ + 0.44 ^2G + 0.05 ^2H
18	Γ_4	75,290	0.30 ^2H + 0.28 ^2P + 0.24 ^2G
19	$\Gamma_{2,3}$	79,031	0.43 $^2D2$ + 0.28 $^2D1$ + 0.15 ^2G
20	Γ_4	89,511	0.68 $^2D1$ + 0.16 ^2F + 0.14 ^2H

[a] *Irreducible representations of the T group, $\Gamma_{2,3} = \Gamma_2 + \Gamma_3$ (Bethe notation, G. F. Koster, J. O. Dimmock, R. G. Wheeler, and H. Statz, Properties of the thirty-two point groups, MIT Press, Cambridge, MA (1963)).*

Table 11. Energy levels (cm^{-1}) for Mn^{4+} using the parameters of tables 2 and 4, for Ge site in $Bi_{12}GeO_{20}$, T symmetry, ζ = 405 cm^{-1}

No.	I.R.[a]	Energy (cm^{-1})	Free ion state				
1	$\Gamma_{6,7}$	0	0.40 ^2G	+	0.32 ^2H	+	0.15 $^2D1$
2	Γ_5	8,034	0.88 ^4F	+	0.12 ^4P		
3	$\Gamma_{6,7}$	8,055	0.88 ^4F	+	0.12 ^4P		
4	$\Gamma_{6,7}$	8,431	0.88 ^4F	+	0.12 ^4P		
5	Γ_5	8,674	0.87 ^4F	+	0.13 ^4P		
6	Γ_5	22,548	0.55 ^2H	+	0.44 ^2G		
7	$\Gamma_{6,7}$	22,771	0.55 ^2H	+	0.44 ^2G	+	0.01 $^2D2$
8	Γ_5	23,534	0.52 ^2G	+	0.24 $^2D2$	+	0.15 ^2H
9	$\Gamma_{6,7}$	23,739	0.50 ^2G	+	0.23 $^2D2$	+	0.18 ^2H
10	Γ_5	26,549	0.54 ^2P	+	0.27 ^2F	+	0.19 ^2H
11	$\Gamma_{6,7}$	26,864	0.54 ^2P	+	0.27 ^2F	+	0.19 ^2H
12	Γ_5	32,310	1.00 ^4F				
13	$\Gamma_{6,7}$	32,426	0.99 ^4F				
14	$\Gamma_{6,7}$	32,566	1.00 ^4F				
15	Γ_5	32,574	1.00 ^4F				
16	$\Gamma_{6,7}$	37,747	0.35 ^2H	+	0.29 ^2F	+	0.24 $^2D1$
17	Γ_5	38,097	0.37 ^2H	+	0.26 ^2F	+	0.24 $^2D1$
18	Γ_5	39,481	0.87 ^4P	+	0.13 ^4F		
19	$\Gamma_{6,7}$	39,642	0.87 ^4P	+	0.12 ^4F		
20	$\Gamma_{6,7}$	39,879	0.87 ^4P	+	0.12 ^4F	+	0.01 ^2H
21	Γ_5	39,925	0.85 ^4P	+	0.11 ^4F	+	0.02 ^2H
22	Γ_5	46,589	1.00 ^2G				
23	Γ_5	48,613	0.63 ^2H	+	0.23 ^2G	+	0.14 ^2P
24	$\Gamma_{6,7}$	48,803	0.58 ^2H	+	0.26 ^2G	+	0.15 ^2P
25	$\Gamma_{6,7}$	49,850	0.41 ^2G	+	0.29 $^2D2$	+	0.17 ^2H
26	Γ_5	49,965	0.42 ^2G	+	0.33 $^2D2$	+	0.13 ^2H
27	$\Gamma_{6,7}$	50,568	0.49 ^2H	+	0.42 $^2D2$	+	0.06 $^2D1$
28	$\Gamma_{6,7}$	53,819	0.54 ^2F	+	0.36 ^2H	+	0.06 ^2G
29	Γ_5	53,962	0.56 ^2F	+	0.32 ^2H	+	0.08 ^2G
30	$\Gamma_{6,7}$	54,674	0.41 $^2D2$	+	0.39 ^2F	+	0.18 ^2H
31	Γ_5	54,746	0.43 ^2F	+	0.37 $^2D2$	+	0.18 ^2H
32	$\Gamma_{6,7}$	58,029	0.99 ^4F				
33	Γ_5	58,038	1.00 ^2F				
34	$\Gamma_{6,7}$	68,125	0.51 $^2D1$	+	0.44 ^2G	+	0.05 ^2H
35	Γ_5	75,294	0.31 ^2H	+	0.27 ^2P	+	0.25 ^2G
36	$\Gamma_{6,7}$	75,380	0.30 ^2H	+	0.28 ^2P	+	0.24 ^2G
37	$\Gamma_{6,7}$	79,098	0.43 $^2D2$	+	0.28 $^2D1$	+	0.15 ^2G
38	Γ_5	89,441	0.68 $^2D1$	+	0.15 ^2F	+	0.15 ^2H
39	$\Gamma_{6,7}$	89,657	0.68 $^2D1$	+	0.16 ^2F	+	0.14 ^2H

[a] *Irreducible representations of the double T (cubic) group (G. F. Koster, J. O. Dimmock, R. G. Wheeler, and H. Statz, Properties of the thirty-two point groups, MIT Press, Cambridge, MA (1963)).*

Table 12. Energy levels (cm^{-1}) for Fe^{4+} using the parameters of tables 2 and 4, for Ge site in $Bi_{12}GeO_{20}$, T symmetry, no spin orbit

No.	I.R.[a]	Energy (cm^{-1})	Free ion state
1	Γ_1	0	0.40 ^1I + 0.30 $^1G1$ + 0.22 $^1G2$
2	Γ_4	45	1.00 ^5D
3	Γ_4	5,601	0.47 ^3H + 0.25 $^3F2$ + 0.15 $^3P1$
4	Γ_4	9,139	0.40 ^3G + 0.27 ^3H + 0.17 $^3F1$
5	Γ_4	14,290	0.62 ^1I + 0.21 $^1G1$ + 0.17 $^1G2$
6	$\Gamma_{2,3}$	16,776	1.00 ^5D
7	Γ_4	19,938	0.67 ^3H + 0.28 $^3F2$ + 0.04 $^3F1$
8	Γ_4	20,554	0.52 ^3H + 0.43 ^3G + 0.04 $^3F2$
9	Γ_4	21,631	0.36 ^1I + 0.20 ^1F + 0.19 $^1D2$
10	$\Gamma_{2,3}$	22,245	0.52 ^3G + 0.30 ^3H + 0.18 ^3D
11	Γ_4	22,983	0.50 ^3G + 0.37 $^3P2$ + 0.05 $^3P1$
12	Γ_4	24,961	0.53 ^3D + 0.43 $^3F2$ + 0.03 ^3G
13	Γ_4	29,791	0.62 ^1I + 0.17 $^1G2$ + 0.11 $^1D2$
14	$\Gamma_{2,3}$	30,722	0.51 $^1G2$ + 0.25 ^1I + 0.17 $^1G1$
15	Γ_1	31,331	0.48 ^1I + 0.28 $^1S2$ + 0.16 $^1G2$
16	Γ_4	33,577	0.52 $^3F1$ + 0.48 $^3F2$
17	Γ_4	34,226	0.43 $^1G2$ + 0.32 ^1F + 0.21 ^1I
18	Γ_1	34,661	0.54 ^1F + 0.46 ^1I
19	Γ_4	35,518	0.52 ^3H + 0.28 $^3F2$ + 0.10 $^3P1$
20	Γ_4	35,647	0.30 $^1D2$ + 0.27 ^1F + 0.25 ^1I
21	$\Gamma_{2,3}$	36,622	0.68 ^3H + 0.30 ^3G + 0.02 ^3D
22	Γ_4	38,743	0.38 $^3F2$ + 0.24 ^3D + 0.20 ^3H
23	$\Gamma_{2,3}$	38,750	1.00 ^3G
24	Γ_4	38,832	0.40 $^3P2$ + 0.35 ^3G + 0.14 $^3F1$
25	$\Gamma_{2,3}$	41,856	0.80 ^3D + 0.18 ^3G + 0.02 ^3H
26	$\Gamma_{2,3}$	43,396	0.45 $^1D2$ + 0.40 $^1G1$ + 0.12 $^1D1$
27	Γ_4	44,946	0.49 ^1I + 0.23 $^1G1$ + 0.21 $^1D2$
28	$\Gamma_{2,3}$	46,774	0.55 ^1I + 0.35 $^1G2$ + 0.03 $^1D1$
29	Γ_4	48,037	0.52 $^3F2$ + 0.48 $^3F1$
30	Γ_1	48,084	0.54 ^1I + 0.46 ^1F
31	Γ_4	50,506	0.47 $^1G2$ + 0.27 ^1F + 0.09 $^1D1$
32	Γ_1	50,732	0.45 $^1G2$ + 0.42 $^1S2$ + 0.09 $^1S1$
33	Γ_4	50,904	0.65 ^1F + 0.13 $^1G2$ + 0.13 ^1I
34	Γ_4	55,156	0.70 $^3P1$ + 0.13 $^3F2$ + 0.08 $^3P2$
35	Γ_4	55,479	0.74 $^3F1$ + 0.11 $^3F2$ + 0.10 ^3D
36	Γ_4	61,956	0.61 $^1G1$ + 0.17 ^1I + 0.09 $^1D2$
37	Γ_4	61,971	0.65 $^3F1$ + 0.14 ^3H + 0.12 ^3G
38	$\Gamma_{2,3}$	64,355	0.50 $^1D1$ + 0.36 $^1D2$ + 0.07 $^1G2$
39	Γ_1	64,403	0.50 $^1G1$ + 0.18 $^1S2$ + 0.14 $^1G2$
40	Γ_4	64,766	0.67 $^1G1$ + 0.26 $^1G2$ + 0.05 ^1I
41	$\Gamma_{2,3}$	73,171	0.34 $^1D1$ + 0.33 $^1G1$ + 0.16 ^1I
42	Γ_4	79,955	0.69 $^1D1$ + 0.14 ^1F + 0.09 $^1D2$
43	Γ_1	100,394	0.72 $^1S1$ + 0.18 $^1G1$ + 0.06 $^1S2$

[a] *Irreducible representations of the T (cubic) group, $\Gamma_{2,3} = \Gamma_2 + \Gamma_3$ (Bethe notation, G. F. Koster, J. O. Dimmock, R. G. Wheeler, and H. Statz, Properties of the thirty-two point groups, MIT Press, Cambridge, MA (1963)).*

Table 13. Energy levels (cm^{-1}) for Fe^{4+} using the parameters of tables 2 and 4, for Ge site in $Bi_{12}GeO_{20}$, T symmetry, ζ = 513 cm^{-1}

No.	I.R.[a]	Energy (cm^{-1})	Free ion state
1	Γ_1	0	0.67 ^5D + 0.11 ^1I + 0.08 $^1G1$
2	Γ_4	159	0.99 ^5D
3	Γ_4	208	0.99 ^5D
4	Γ_1	354	0.31 ^5D + 0.27 ^1I + 0.20 $^1G1$
5	$\Gamma_{2,3}$	579	0.99 ^5D
6	Γ_4	606	1.00 ^5D
7	Γ_4	868	1.00 ^5D
8	Γ_4	5,962	0.47 ^3H + 0.24 $^3F2$ + 0.15 $^3P1$
9	Γ_1	6,007	0.44 ^3H + 0.22 $^3F2$ + 0.15 $^3P1$
10	$\Gamma_{2,3}$	6,196	0.47 ^3H + 0.26 $^3F2$ + 0.14 $^3P1$
11	Γ_4	6,253	0.47 ^3H + 0.26 $^3F2$ + 0.14 $^3P1$
12	Γ_1	9,214	0.44 ^3G + 0.24 ^3H + 0.17 $^3F1$
13	Γ_4	9,430	0.42 ^3G + 0.26 ^3H + 0.17 $^3F1$
14	Γ_4	9,760	0.38 ^3G + 0.29 ^3H + 0.16 $^3F1$
15	$\Gamma_{2,3}$	9,838	0.38 ^3G + 0.29 ^3H + 0.16 $^3F1$
16	Γ_4	14,690	0.60 ^1I + 0.21 $^1G1$ + 0.17 $^1G2$
17	Γ_1	17,147	0.97 ^5D + 0.01 ^3H + 0.01 $^3F2$
18	Γ_4	17,164	0.98 ^5D + 0.01 ^3H + 0.01 $^3F2$
19	$\Gamma_{2,3}$	17,174	0.98 ^5D + 0.01 ^3H + 0.01 $^3F2$
20	Γ_4	17,183	0.99 ^5D
21	Γ_1	17,193	0.99 ^5D
22	$\Gamma_{2,3}$	20,302	0.65 ^3H + 0.22 $^3F2$ + 0.09 ^3G
23	Γ_4	20,387	0.66 ^3H + 0.25 $^3F2$ + 0.04 ^3G
24	Γ_1	20,410	0.65 ^3H + 0.29 $^3F2$ + 0.04 $^3F1$
25	Γ_4	20,433	0.64 ^3H + 0.26 $^3F2$ + 0.04 ^3G
26	Γ_4	21,055	0.51 ^3H + 0.41 ^3G + 0.07 $^3F2$
27	Γ_1	21,061	0.55 ^3H + 0.41 ^3G + 0.03 $^3F2$
28	Γ_4	21,064	0.53 ^3H + 0.37 ^3G + 0.07 $^3F2$
29	$\Gamma_{2,3}$	21,174	0.53 ^3H + 0.36 ^3G + 0.10 $^3F2$
30	Γ_4	21,813	0.27 ^1I + 0.15 ^1F + 0.15 $^1D2$
31	Γ_4	22,725	0.51 ^3G + 0.31 ^3H + 0.18 ^3D
32	Γ_4	22,884	0.43 ^3G + 0.25 ^3H + 0.15 ^3D
33	Γ_1	23,358	0.46 ^3G + 0.37 $^3P2$ + 0.06 ^3H
34	Γ_4	23,413	0.48 ^3G + 0.37 $^3P2$ + 0.05 ^3H
35	$\Gamma_{2,3}$	23,506	0.51 ^3G + 0.36 $^3P2$ + 0.05 $^3P1$
36	Γ_4	23,545	0.50 ^3G + 0.36 $^3P2$ + 0.05 $^3P1$
37	Γ_1	25,473	0.54 ^3D + 0.43 $^3F2$ + 0.02 ^3G
38	$\Gamma_{2,3}$	25,479	0.51 ^3D + 0.43 $^3F2$ + 0.05 ^3G
39	Γ_4	25,484	0.52 ^3D + 0.43 $^3F2$ + 0.05 ^3G
40	Γ_4	25,535	0.51 ^3D + 0.42 $^3F2$ + 0.03 ^3G
41	Γ_4	30,220	0.61 ^1I + 0.17 $^1G2$ + 0.11 $^1D2$
42	$\Gamma_{2,3}$	31,154	0.50 $^1G2$ + 0.25 ^1I + 0.17 $^1G1$
43	Γ_1	31,733	0.47 ^1I + 0.27 $^1S2$ + 0.16 $^1G2$
44	Γ_4	34,103	0.52 $^3F1$ + 0.47 $^3F2$
45	Γ_4	34,531	0.39 $^1G2$ + 0.30 ^1F + 0.19 ^1I
46	Γ_1	35,089	0.53 ^1F + 0.45 ^1I + 0.01 $^3F2$
47	Γ_4	35,924	0.34 ^3H + 0.17 $^3F2$ + 0.11 ^1F
48	$\Gamma_{2,3}$	35,984	0.51 ^3H + 0.29 $^3F2$ + 0.10 $^3P1$
49	Γ_4	36,060	0.19 $^1D2$ + 0.19 ^3H + 0.15 ^1F

Table 13. Energy levels (cm^{-1}) for Fe^{4+} using the parameters of tables 2 and 4, for Ge site in $Bi_{12}GeO_{20}$, T symmetry, ζ = 513 cm^{-1} (cont'd)

No.	I.R.[a]	Energy (cm^{-1})	Free ion state				
50	Γ_1	36,127	0.52 ^3H	+	0.27 $^3F2$	+	0.10 $^3P1$
51	Γ_4	36,138	0.49 ^3H	+	0.26 $^3F2$	+	0.09 $^3P1$
52	Γ_4	37,135	0.67 ^3H	+	0.29 ^3G	+	0.02 ^3D
53	Γ_4	37,170	0.66 ^3H	+	0.28 ^3G	+	0.02 ^3D
54	Γ_4	39,070	0.31 $^3F2$	+	0.18 ^3D	+	0.17 ^3H
55	$\Gamma_{2,3}$	39,088	0.35 $^3F2$	+	0.21 ^3D	+	0.20 ^3H
56	Γ_4	39,172	0.64 ^3G	+	0.12 $^3P2$	+	0.07 $^3F2$
57	Γ_1	39,179	0.38 ^3G	+	0.37 $^3P2$	+	0.15 $^3F1$
58	Γ_4	39,358	0.25 $^3P2$	+	0.24 ^3G	+	0.16 $^3F2$
59	Γ_4	39,377	0.63 ^3G	+	0.20 $^3P2$	+	0.07 $^3F1$
60	$\Gamma_{2,3}$	39,418	0.38 $^3P2$	+	0.30 ^3G	+	0.14 $^3F1$
61	Γ_4	39,483	0.24 $^3F2$	+	0.17 ^3G	+	0.17 $^3P2$
62	Γ_1	39,590	0.38 $^3F2$	+	0.25 ^3D	+	0.19 ^3H
63	Γ_4	42,346	0.79 ^3D	+	0.18 ^3G	+	0.02 ^3H
64	Γ_4	42,348	0.80 ^3D	+	0.18 ^3G	+	0.02 ^3H
65	$\Gamma_{2,3}$	43,871	0.44 $^1D2$	+	0.39 $^1G1$	+	0.12 $^1D1$
66	Γ_4	45,448	0.49 ^1I	+	0.23 $^1G1$	+	0.21 $^1D2$
67	$\Gamma_{2,3}$	47,259	0.55 ^1I	+	0.35 $^1G2$	+	0.04 $^1D1$
68	Γ_4	48,532	0.52 $^3F2$	+	0.48 $^3F1$		
69	Γ_1	48,545	0.54 ^1I	+	0.46 ^1F		
70	Γ_4	50,955	0.47 $^1G2$	+	0.27 ^1F	+	0.09 $^1D1$
71	Γ_1	51,112	0.44 $^1G2$	+	0.41 $^1S2$	+	0.08 $^1S1$
72	Γ_4	51,359	0.64 ^1F	+	0.13 $^1G2$	+	0.13 ^1I
73	$\Gamma_{2,3}$	55,463	0.67 $^3P1$	+	0.14 $^3F2$	+	0.07 ^3H
74	Γ_4	55,471	0.68 $^3P1$	+	0.14 $^3F2$	+	0.07 ^3H
75	Γ_1	55,822	0.74 $^3F1$	+	0.10 $^3F2$	+	0.08 ^3D
76	Γ_4	55,839	0.66 $^3P1$	+	0.13 $^3F2$	+	0.09 $^3P2$
77	Γ_4	55,926	0.72 $^3F1$	+	0.11 $^3F2$	+	0.09 ^3D
78	$\Gamma_{2,3}$	56,104	0.70 $^3F1$	+	0.11 $^3F2$	+	0.10 ^3D
79	Γ_4	56,129	0.69 $^3F1$	+	0.11 $^3F2$	+	0.10 ^3D
80	Γ_1	56,168	0.67 $^3P1$	+	0.12 $^3F2$	+	0.09 $^3P2$
81	Γ_4	62,162	0.37 $^1G1$	+	0.26 $^3F1$	+	0.11 ^1I
82	Γ_1	62,219	0.66 $^3F1$	+	0.14 ^3H	+	0.11 ^3G
83	Γ_4	62,378	0.66 $^3F1$	+	0.14 ^3H	+	0.12 ^3G
84	$\Gamma_{2,3}$	62,590	0.64 $^3F1$	+	0.14 ^3H	+	0.13 ^3G
85	Γ_4	62,963	0.39 $^3F1$	+	0.24 $^1G1$	+	0.09 ^3H
86	$\Gamma_{2,3}$	64,886	0.49 $^1D1$	+	0.35 $^1D2$	+	0.07 $^1G2$
87	Γ_1	64,921	0.50 $^1G1$	+	0.18 $^1S2$	+	0.14 $^1G2$
88	Γ_4	65,279	0.67 $^1G1$	+	0.26 $^1G2$	+	0.04 ^1I
89	$\Gamma_{2,3}$	73,700	0.33 $^1D1$	+	0.33 $^1G1$	+	0.16 ^1I
90	Γ_4	80,458	0.69 $^1D1$	+	0.14 ^1F	+	0.09 $^1D2$
91	Γ_1	100,908	0.72 $^1S1$	+	0.18 $^1G1$	+	0.06 $^1S2$

[a] *Irreducible representations of the T (cubic) group, $\Gamma_{2,3} = \Gamma_2 + \Gamma_3$ (G. F. Koster, J. O. Dimmock, R. G. Wheeler, and H. Statz, Properties of the thirty-two point groups, MIT Press, Cambridge, MA (1963)).*

Table 14. Energy levels (cm^{-1}) for Co^{4+} using the parameters of tables 2 and 4, for Ge site in $Bi_{12}GeO_{20}$, T symmetry, no spin orbit

No.	I.R.[a]	Energy (cm^{-1})	Free ion state
1	Γ_1	0	1.00 ^6S
2	Γ_4	17,382	0.63 ^4G + 0.33 ^4P + 0.03 ^4F
3	Γ_4	21,309	0.35 ^2I + 0.26 ^2H + 0.17 $^2F1$
4	Γ_4	21,316	0.50 ^4G + 0.26 ^4F + 0.24 ^4D
5	Γ_4	28,043	1.00 ^4G
6	Γ_4	30,284	0.57 ^4D + 0.41 ^4G + 0.02 ^4F
7	Γ_1	31,705	0.59 ^2I + 0.37 $^2F1$ + 0.04 $^2F2$
8	Γ_4	31,834	0.63 ^2I + 0.23 ^2H + 0.12 $^2F1$
9	$\Gamma_{2,3}$	32,470	1.00 ^4D
10	Γ_4	33,261	0.52 ^2I + 0.22 $^2F1$ + 0.10 ^2H
11	$\Gamma_{2,3}$	35,005	0.43 ^2I + 0.25 ^2H + 0.12 $^2D3$
12	Γ_4	38,873	0.37 $^2G2$ + 0.20 $^2F2$ + 0.18 $^2F1$
13	Γ_1	40,501	0.71 ^2I + 0.15 $^2G2$ + 0.10 $^2G1$
14	Γ_4	40,547	0.32 $^2G2$ + 0.24 $^2F2$ + 0.18 ^2I
15	Γ_4	41,108	0.45 ^4P + 0.43 ^4F + 0.11 ^4G
16	$\Gamma_{2,3}$	43,278	0.45 ^2I + 0.29 $^2D3$ + 0.11 ^2H
17	Γ_1	43,831	0.51 $^2G2$ + 0.28 ^2I + 0.12 $^2G1$
18	Γ_4	44,300	0.45 ^2I + 0.39 $^2D3$ + 0.06 $^2D1$
19	Γ_1	44,320	1.00 ^4F
20	$\Gamma_{2,3}$	47,294	0.73 $^2G2$ + 0.12 $^2D3$ + 0.05 $^2D1$
21	Γ_4	48,545	0.46 $^2F2$ + 0.27 $^2G2$ + 0.12 ^2I
22	Γ_4	48,708	0.53 ^4F + 0.26 ^4G + 0.21 ^4P
23	Γ_1	49,327	0.75 $^2F2$ + 0.18 ^2I + 0.07 $^2F1$
24	Γ_4	49,402	0.52 $^2F2$ + 0.37 $^2G2$ + 0.07 ^2I
25	Γ_4	51,107	0.68 ^2H + 0.31 $^2F1$
26	Γ_1	52,702	0.71 ^2S + 0.24 $^2G2$ + 0.04 $^2G1$
27	Γ_4	53,233	0.71 ^4F + 0.19 ^4D + 0.10 ^4G
28	$\Gamma_{2,3}$	55,188	0.44 ^2H + 0.30 $^2D3$ + 0.24 $^2D2$
29	Γ_4	56,796	0.41 ^2H + 0.20 $^2F1$ + 0.16 $^2F2$
30	Γ_4	58,217	0.34 $^2F1$ + 0.22 ^2H + 0.13 $^2G2$
31	Γ_4	61,526	0.45 ^2H + 0.27 ^2I + 0.18 $^2F1$
32	Γ_1	61,634	0.56 $^2F1$ + 0.23 ^2I + 0.21 $^2F2$
33	$\Gamma_{2,3}$	64,912	0.78 $^2G1$ + 0.08 ^2H + 0.07 $^2D1$
34	Γ_4	67,311	0.49 $^2D2$ + 0.17 $^2G1$ + 0.13 ^2I
35	$\Gamma_{2,3}$	68,375	0.60 $^2D2$ + 0.10 ^2H + 0.10 $^2G2$
36	Γ_4	69,487	0.26 $^2D3$ + 0.22 ^2H + 0.18 $^2F1$
37	Γ_4	70,166	0.80 $^2G1$ + 0.07 ^2P + 0.06 $^2F2$
38	Γ_4	73,792	0.52 $^2G1$ + 0.13 $^2F2$ + 0.12 $^2G2$
39	Γ_1	75,794	0.74 $^2G1$ + 0.16 ^2S + 0.10 $^2G2$
40	Γ_4	80,636	0.87 ^2P + 0.04 $^2F2$ + 0.04 $^2G2$
41	Γ_4	94,481	0.73 $^2D1$ + 0.07 ^2H + 0.05 $^2D3$
42	$\Gamma_{2,3}$	94,533	0.73 $^2D1$ + 0.10 $^2G1$ + 0.10 $^2D3$

[a] *Irreducible representations of the T (cubic) group, $\Gamma_{2,3} = \Gamma_2 + \Gamma_3$ (Bethe notation, G. F. Koster, J. O. Dimmock, R. G. Wheeler, and H. Statz, Properties of the thirty-two point groups, MIT Press, Cambridge, MA (1963)).*

Table 15. Energy levels (cm^{-1}) for Co^{4+} using the parameters of tables 2 and 4, for Ge site in $Bi_{12}GeO_{20}$, T symmetry, ζ = 654 cm^{-1}

No.	I.R.[a]	Energy (cm^{-1})	Free ion state
1	$\Gamma_{6,7}$	0	1.00 ^6S
2	$\Gamma_{6,7}$	0.04	1.00 ^6S
3	Γ_5	17,231	0.63 ^4G + 0.33 ^4P + 0.04 ^4F
4	$\Gamma_{6,7}$	17,247	0.61 ^4G + 0.32 ^4P + 0.04 ^4F
5	Γ_5	17,313	0.60 ^4G + 0.32 ^4P + 0.03 ^4F
6	$\Gamma_{6,7}$	17,410	0.61 ^4G + 0.33 ^4P + 0.03 ^4F
7	$\Gamma_{6,7}$	20,762	0.22 ^4G + 0.19 ^2I + 0.14 ^2H
8	Γ_5	21,241	0.43 ^4G + 0.26 ^4D + 0.25 ^4F
9	Γ_5	21,350	0.53 ^4G + 0.26 ^4F + 0.21 ^4D
10	$\Gamma_{6,7}$	21,374	0.53 ^4G + 0.26 ^4F + 0.21 ^4D
11	$\Gamma_{6,7}$	21,689	0.29 ^4G + 0.16 ^4F + 0.16 ^4D
12	Γ_5	22,297	0.34 ^2I + 0.25 ^2H + 0.13 $^2F1$
13	$\Gamma_{6,7}$	27,957	0.97 ^4G + 0.01 ^2I + 0.01 $^2F1$
14	Γ_5	27,995	0.98 ^4G + 0.01 $^2F1$
15	Γ_5	28,019	0.98 ^4G + 0.01 ^2I + 0.01 ^2H
16	$\Gamma_{6,7}$	28,052	0.99 ^4G
17	Γ_5	29,754	0.46 ^4D + 0.40 ^4G + 0.06 ^2I
18	$\Gamma_{6,7}$	30,194	0.54 ^4D + 0.43 ^4G + 0.02 ^4F
19	$\Gamma_{6,7}$	30,416	0.59 ^4D + 0.37 ^4G + 0.02 ^4F
20	Γ_5	30,468	0.60 ^4D + 0.37 ^4G + 0.02 ^4F
21	Γ_5	31,558	0.60 ^2I + 0.22 ^2H + 0.10 $^2F1$
22	$\Gamma_{6,7}$	32,017	0.52 ^2I + 0.18 ^2H + 0.14 ^4D
23	$\Gamma_{6,7}$	32,053	0.53 ^2I + 0.31 $^2F1$ + 0.07 ^4G
24	Γ_5	32,341	0.90 ^4D + 0.05 ^2I + 0.02 $^2F1$
25	$\Gamma_{6,7}$	32,515	0.81 ^4D + 0.12 ^2I + 0.04 ^2H
26	Γ_5	32,554	0.96 ^4D + 0.02 ^2I + 0.01 ^2H
27	$\Gamma_{6,7}$	33,427	0.49 ^2I + 0.20 $^2F1$ + 0.10 ^2H
28	Γ_5	33,591	0.48 ^2I + 0.20 $^2F1$ + 0.10 ^4D
29	$\Gamma_{6,7}$	35,102	0.43 ^2I + 0.25 ^2H + 0.12 $^2D3$
30	Γ_5	38,794	0.39 $^2G2$ + 0.20 $^2F1$ + 0.16 $^2F2$
31	$\Gamma_{6,7}$	38,807	0.34 $^2G2$ + 0.20 $^2F2$ + 0.16 ^2H
32	Γ_5	40,366	0.41 ^2I + 0.15 ^4F + 0.15 ^4P
33	Γ_5	40,399	0.28 $^2F2$ + 0.25 $^2G2$ + 0.11 $^2D2$
34	$\Gamma_{6,7}$	40,492	0.29 $^2G2$ + 0.21 $^2F2$ + 0.16 ^2I
35	Γ_5	41,114	0.30 ^4P + 0.30 ^2I + 0.26 ^4F
36	$\Gamma_{6,7}$	41,115	0.39 ^4P + 0.39 ^4F + 0.11 ^4G
37	$\Gamma_{6,7}$	41,246	0.40 ^4P + 0.36 ^4F + 0.10 ^4G
38	Γ_5	41,368	0.38 ^4P + 0.36 ^4F + 0.10 ^4G
39	$\Gamma_{6,7}$	43,563	0.42 ^2I + 0.26 $^2D3$ + 0.10 ^2H
40	Γ_5	43,935	0.50 $^2G2$ + 0.26 ^2I + 0.12 $^2G1$
41	$\Gamma_{6,7}$	44,070	0.44 ^4F + 0.28 ^2I + 0.19 $^2D3$
42	Γ_5	44,497	0.43 ^2I + 0.39 $^2D3$ + 0.06 $^2D1$
43	$\Gamma_{6,7}$	44,820	0.55 ^4F + 0.18 $^2D3$ + 0.15 ^2I
44	$\Gamma_{6,7}$	47,236	0.66 $^2G2$ + 0.12 $^2D3$ + 0.05 ^4F
45	Γ_5	47,676	0.25 $^2F2$ + 0.20 ^4F + 0.18 $^2G2$
46	$\Gamma_{6,7}$	48,127	0.26 ^4F + 0.23 $^2F2$ + 0.14 ^4G
47	$\Gamma_{6,7}$	48,789	0.48 ^4F + 0.22 ^4G + 0.18 ^4P
48	Γ_5	49,092	0.52 ^4F + 0.24 ^4G + 0.18 ^4P
49	$\Gamma_{6,7}$	49,185	0.30 $^2F2$ + 0.23 $^2G2$ + 0.17 ^4F

Table 15. Energy levels (cm^{-1}) for Co^{4+} using the parameters of tables 2 and 4, for Ge site in $Bi_{12}GeO_{20}$, T symmetry, ζ = 654 cm^{-1} (cont'd)

No.	I.R.[a]	Energy (cm^{-1})	Free ion state				
50	Γ_5	49,222	0.41 $^2F2$	+	0.19 ^4F	+	0.12 ^2I
51	$\Gamma_{6,7}$	49,356	0.43 $^2F2$	+	0.29 $^2G2$	+	0.09 ^4F
52	Γ_5	49,398	0.49 $^2F2$	+	0.14 ^4F	+	0.12 ^2I
53	Γ_5	49,442	0.54 $^2F2$	+	0.30 $^2G2$	+	0.06 ^2I
54	Γ_5	51,355	0.66 ^2H	+	0.24 $^2F1$	+	0.03 ^4F
55	$\Gamma_{6,7}$	51,366	0.63 ^2H	+	0.29 $^2F1$	+	0.02 ^4F
56	Γ_5	52,896	0.67 2S	+	0.24 $^2G2$	+	0.04 $^2G1$
57	$\Gamma_{6,7}$	53,152	0.68 ^4F	+	0.17 ^4D	+	0.10 ^4G
58	Γ_5	53,301	0.67 ^4F	+	0.16 ^4D	+	0.10 ^4G
59	$\Gamma_{6,7}$	53,417	0.69 ^4F	+	0.19 ^4D	+	0.09 ^4G
60	Γ_5	53,697	0.69 ^4F	+	0.20 ^4D	+	0.08 ^4G
61	$\Gamma_{6,7}$	55,364	0.42 ^2H	+	0.30 $^2D3$	+	0.22 $^2D2$
62	$\Gamma_{6,7}$	56,870	0.42 ^2H	+	0.18 $^2F1$	+	0.16 $^2F2$
63	Γ_5	57,054	0.35 ^2H	+	0.24 $^2F1$	+	0.14 $^2F2$
64	Γ_5	58,351	0.36 $^2F1$	+	0.20 ^2H	+	0.14 $^2G2$
65	$\Gamma_{6,7}$	58,452	0.32 $^2F1$	+	0.23 ^2H	+	0.12 $^2G2$
66	$\Gamma_{6,7}$	61,535	0.44 ^2H	+	0.26 ^2I	+	0.18 $^2F1$
67	Γ_5	61,781	0.56 $^2F1$	+	0.22 ^2I	+	0.20 $^2F2$
68	Γ_5	61,964	0.46 ^2H	+	0.27 ^2I	+	0.16 $^2F1$
69	$\Gamma_{6,7}$	65,000	0.78 $^2G1$	+	0.08 ^2H	+	0.07 $^2D1$
70	Γ_5	67,382	0.43 $^2D2$	+	0.20 $^2G1$	+	0.14 ^2I
71	$\Gamma_{6,7}$	67,414	0.52 $^2D2$	+	0.15 $^2G1$	+	0.13 ^2I
72	$\Gamma_{6,7}$	68,498	0.59 $^2D2$	+	0.10 ^2H	+	0.10 $^2G2$
73	Γ_5	69,282	0.25 $^2D3$	+	0.22 ^2H	+	0.18 $^2F1$
74	$\Gamma_{6,7}$	69,813	0.26 $^2D3$	+	0.21 ^2H	+	0.17 $^2F1$
75	Γ_5	70,063	0.81 $^2G1$	+	0.07 ^2P	+	0.05 $^2F2$
76	$\Gamma_{6,7}$	70,392	0.78 $^2G1$	+	0.08 ^2P	+	0.06 $^2F2$
77	Γ_5	73,826	0.52 $^2G1$	+	0.15 $^2F2$	+	0.10 $^2G2$
78	$\Gamma_{6,7}$	73,964	0.51 $^2G1$	+	0.13 $^2G2$	+	0.11 $^2F2$
79	Γ_5	75,894	0.74 $^2G1$	+	0.15 2S	+	0.10 $^2G2$
80	$\Gamma_{6,7}$	80,716	0.87 ^2P	+	0.05 $^2F2$	+	0.04 $^2G2$
81	Γ_5	80,738	0.87 ^2P	+	0.04 $^2G2$	+	0.04 $^2F2$
82	$\Gamma_{6,7}$	94,583	0.73 $^2D1$	+	0.07 $^2D3$	+	0.07 $^2G1$
83	Γ_5	94,621	0.72 $^2D1$	+	0.07 ^2H	+	0.06 $^2D3$
84	$\Gamma_{6,7}$	94,712	0.73 $^2D1$	+	0.08 $^2G1$	+	0.08 $^2D3$

[a] *Irreducible representations of the double T (cubic) group (G. F. Koster, J. O. Dimmock, R. G. Wheeler, and H. Statz, Properties of the thirty-two point groups, MIT Press, Cambridge, MA (1963)).*

Table 16. Energy levels (cm^{-1}) for Ni^{4+} using the parameters of tables 2 and 4, for Ge site in $Bi_{12}GeO_{20}$, T symmetry, no spin orbit

No.	I.R.[a]	Energy (cm^{-1})	Free ion state
1	$\Gamma_{2,3}$	0	1.00 ^5D
2	Γ_4	11,676	1.00 ^5D
3	Γ_4	12,590	0.47 ^3H + 0.17 ^3G + 0.13 $^3F2$
4	$\Gamma_{2,3}$	21,226	0.87 ^3H + 0.12 ^3G + 0.01 ^3D
5	Γ_4	22,495	0.42 ^3H + 0.28 ^3G + 0.20 $^3P2$
6	Γ_4	23,138	0.42 $^3F2$ + 0.38 ^3H + 0.08 $^3F1$
7	Γ_4	23,808	0.44 ^1I + 0.27 $^1G2$ + 0.17 $^1G1$
8	Γ_1	23,880	1.00 ^3G
9	$\Gamma_{2,3}$	24,316	0.70 ^1I + 0.16 $^1D2$ + 0.07 $^1G1$
10	Γ_1	24,510	0.94 $^3F2$ + 0.06 $^3F1$
11	$\Gamma_{2,3}$	26,499	0.49 ^3G + 0.48 ^3D + 0.04 ^3H
12	Γ_1	31,376	0.32 ^1I + 0.24 $^1G1$ + 0.23 $^1S2$
13	Γ_4	31,437	0.55 ^3H + 0.32 ^3G + 0.09 $^3P1$
14	Γ_1	32,026	0.94 ^1I + 0.06 ^1F
15	Γ_4	32,626	0.57 ^1I + 0.27 $^1G2$ + 0.07 $^1G1$
16	Γ_4	33,069	0.37 ^3G + 0.35 ^3H + 0.10 $^3F1$
17	Γ_4	33,922	0.40 $^3F2$ + 0.28 ^3H + 0.12 ^3G
18	Γ_4	34,628	0.44 ^1I + 0.29 $^1G2$ + 0.14 ^1F
19	Γ_4	36,016	0.48 ^3D + 0.23 ^3H + 0.15 $^3F2$
20	$\Gamma_{2,3}$	36,226	0.47 $^1D2$ + 0.34 $^1G2$ + 0.11 ^1I
21	$\Gamma_{2,3}$	36,905	0.52 ^3D + 0.39 ^3G + 0.10 ^3H
22	Γ_4	37,571	0.44 ^3G + 0.27 ^3D + 0.27 $^3F2$
23	Γ_4	40,383	0.50 $^3P2$ + 0.27 $^3F2$ + 0.14 ^3H
24	Γ_4	43,140	0.87 ^1I + 0.11 $^1G2$ + 0.02 $^1G1$
25	Γ_1	44,491	0.37 ^1I + 0.32 $^1S2$ + 0.21 $^1G2$
26	Γ_4	45,239	0.43 ^1F + 0.30 ^1I + 0.18 $^1G2$
27	$\Gamma_{2,3}$	45,314	0.48 $^1G2$ + 0.18 $^1G1$ + 0.18 ^1I
28	Γ_4	46,520	0.69 ^1F + 0.12 $^1D1$ + 0.08 $^1G1$
29	Γ_1	48,325	0.57 $^1G2$ + 0.20 $^1S2$ + 0.10 $^1G1$
30	Γ_1	51,292	0.94 ^1F + 0.06 ^1I
31	Γ_4	51,301	0.73 $^1D2$ + 0.09 $^1G1$ + 0.08 ^1F
32	Γ_4	51,464	0.51 $^1G2$ + 0.42 ^1F + 0.06 ^1I
33	Γ_4	53,601	0.70 $^3F1$ + 0.16 $^3P1$ + 0.10 ^3H
34	Γ_1	57,595	0.94 $^3F1$ + 0.06 $^3F2$
35	Γ_4	58,214	0.53 $^3P1$ + 0.17 $^3F2$ + 0.14 $^3P2$
36	Γ_4	60,295	0.70 $^3F1$ + 0.11 ^3D + 0.10 ^3G
37	Γ_4	63,745	0.77 $^1G1$ + 0.20 ^1I + 0.02 $^1G2$
38	$\Gamma_{2,3}$	63,749	0.74 $^1G1$ + 0.17 $^1G2$ + 0.07 $^1D2$
39	Γ_1	69,390	0.51 $^1G1$ + 0.24 ^1I + 0.17 $^1S2$
40	Γ_4	70,055	0.54 $^1G1$ + 0.29 $^1G2$ + 0.10 $^1D2$
41	Γ_4	76,978	0.75 $^1D1$ + 0.11 ^1F + 0.06 $^1D2$
42	$\Gamma_{2,3}$	79,827	0.84 $^1D1$ + 0.16 $^1D2$
43	Γ_1	102,985	0.83 $^1S1$ + 0.09 $^1S2$ + 0.08 $^1G1$

[a] *Irreducible representations of the T (cubic) group, $\Gamma_{2,3} = \Gamma_2 + \Gamma_3$ (Bethe notation, G. F. Koster, J. O. Dimmock, R. G. Wheeler, and H. Statz, Properties of the thirty-two point groups, MIT Press, Cambridge, MA (1963)).*

Table 17. Energy levels (cm^{-1}) for Ni^{4+} using the parameters of tables 2 and 4, for Ge site in $Bi_{12}GeO_{20}$, T symmetry, ζ = 830 cm^{-1}

No.	I.R.[a]	Energy (cm^{-1})	Free ion state
1	Γ_1	0	0.99 ^5D
2	Γ_4	37	0.99 ^5D
3	$\Gamma_{2,3}$	72	0.99 ^5D
4	Γ_4	124	1.00 ^5D
5	Γ_1	176	1.00 ^5D
6	Γ_4	11,142	0.99 ^5D + 0.01 $^3F2$
7	Γ_4	11,598	0.99 ^5D
8	$\Gamma_{2,3}$	11,599	0.99 ^5D
9	Γ_4	12,185	0.84 ^5D + 0.06 ^3H + 0.03 ^3G
10	Γ_4	12,230	0.99 ^5D
11	Γ_1	12,247	0.99 ^5D
12	Γ_4	12,400	0.38 ^3H + 0.15 ^3G + 0.15 ^5D
13	$\Gamma_{2,3}$	12,425	0.43 ^3H + 0.19 ^3G + 0.12 $^3F2$
14	Γ_4	13,069	0.51 ^3H + 0.14 ^3G + 0.13 $^3F2$
15	Γ_1	13,283	0.55 ^3H + 0.13 $^3F2$ + 0.12 ^3G
16	Γ_4	21,211	0.78 ^3H + 0.11 ^3G + 0.02 $^1G2$
17	Γ_4	21,327	0.86 ^3H + 0.13 ^3G + 0.01 ^3D
18	Γ_4	21,985	0.41 ^3H + 0.19 ^3G + 0.16 $^3P2$
19	$\Gamma_{2,3}$	22,258	0.47 ^3H + 0.21 ^3G + 0.19 $^3P2$
20	$\Gamma_{2,3}$	22,738	0.29 $^3F2$ + 0.27 ^3H + 0.18 ^1I
21	Γ_4	22,802	0.36 ^3H + 0.31 $^3F2$ + 0.09 ^3G
22	Γ_1	22,857	0.40 $^3F2$ + 0.37 ^3H + 0.09 $^3F1$
23	Γ_4	23,071	0.36 ^3H + 0.34 ^3G + 0.18 $^3P2$
24	Γ_1	23,508	0.39 ^3G + 0.31 ^3H + 0.20 $^3P2$
25	Γ_4	23,668	0.39 $^3F2$ + 0.38 ^3H + 0.07 $^3F1$
26	Γ_4	23,960	0.97 ^3G + 0.02 ^3H
27	Γ_4	24,171	0.46 $^3F2$ + 0.13 ^1I + 0.12 ^3H
28	Γ_4	25,281	0.53 $^3F2$ + 0.19 ^1I + 0.08 $^1G2$
29	$\Gamma_{2,3}$	25,307	0.50 ^1I + 0.13 $^3F2$ + 0.11 ^3H
30	Γ_4	26,669	0.48 ^3G + 0.46 ^3D + 0.05 ^3H
31	Γ_4	26,735	0.45 ^3D + 0.44 ^3G + 0.06 ^3H
32	Γ_1	30,260	0.25 ^3H + 0.20 ^3G + 0.13 ^1I
33	Γ_4	31,308	0.44 ^3H + 0.22 ^3G + 0.13 ^1I
34	Γ_4	31,620	0.55 ^3H + 0.30 ^3G + 0.10 $^3P1$
35	$\Gamma_{2,3}$	31,780	0.56 ^3H + 0.31 ^3G + 0.07 $^3P1$
36	Γ_1	31,787	0.68 ^1I + 0.12 ^3H + 0.08 ^3G
37	Γ_4	32,578	0.27 ^3H + 0.26 ^3G + 0.16 ^1I
38	Γ_4	32,789	0.41 ^3H + 0.17 ^1I + 0.11 $^1G1$
39	$\Gamma_{2,3}$	33,217	0.34 ^3G + 0.25 ^3H + 0.20 $^3F2$
40	Γ_4	33,309	0.29 ^3H + 0.28 ^3G + 0.12 ^3D
41	Γ_1	33,333	0.29 ^3H + 0.26 ^3G + 0.23 ^1I
42	Γ_4	33,701	0.25 ^3G + 0.20 ^3H + 0.17 ^1I
43	$\Gamma_{2,3}$	33,772	0.23 ^3H + 0.21 ^3G + 0.20 $^3F2$
44	Γ_4	33,972	0.33 $^3F2$ + 0.18 ^3H + 0.15 ^3G
45	Γ_4	34,191	0.29 ^3H + 0.28 $^3F2$ + 0.11 ^3G
46	Γ_1	34,422	0.43 $^3F2$ + 0.23 ^3H + 0.09 ^3G
47	Γ_4	35,094	0.23 ^1I + 0.15 $^1G2$ + 0.12 ^3G
48	$\Gamma_{2,3}$	35,521	0.31 ^3D + 0.22 ^3H + 0.15 $^3F2$
49	Γ_4	36,073	0.49 ^3D + 0.26 ^3H + 0.10 $^3F2$

Table 17. Energy levels (cm^{-1}) for Ni^{4+} using the parameters of tables 2 and 4, for Ge site in $Bi_{12}GeO_{20}$, T symmetry, ζ = 830 cm^{-1} (cont'd)

No.	I.R.[a]	Energy (cm^{-1})	Free ion state				
50	Γ_4	36,433	0.44 ^3D	+	0.21 ^3H	+	0.17 $^3F2$
51	Γ_1	36,794	0.41 ^3D	+	0.19 ^3H	+	0.18 $^3F2$
52	Γ_4	37,126	0.48 ^3D	+	0.41 ^3G	+	0.10 ^3H
53	$\Gamma_{2,3}$	37,175	0.27 $^1D2$	+	0.23 $^1G2$	+	0.13 ^3H
54	Γ_4	37,236	0.42 ^3D	+	0.39 ^3G	+	0.08 ^3H
55	$\Gamma_{2,3}$	37,483	0.46 ^3G	+	0.25 $^3F2$	+	0.24 ^3D
56	Γ_4	37,610	0.41 ^3G	+	0.28 $^3F2$	+	0.22 ^3D
57	Γ_4	38,191	0.39 ^3G	+	0.32 ^3D	+	0.26 $^3F2$
58	Γ_1	38,510	0.37 ^3G	+	0.37 ^3D	+	0.25 $^3F2$
59	Γ_4	40,349	0.44 $^3P2$	+	0.31 $^3F2$	+	0.15 ^3H
60	$\Gamma_{2,3}$	40,430	0.40 $^3P2$	+	0.32 $^3F2$	+	0.14 ^3H
61	Γ_4	41,018	0.55 $^3P2$	+	0.22 $^3F2$	+	0.12 ^3H
62	Γ_1	41,129	0.55 $^3P2$	+	0.19 $^3F2$	+	0.12 ^3G
63	Γ_4	43,447	0.86 ^1I	+	0.11 $^1G2$	+	0.02 $^1G1$
64	Γ_1	44,917	0.35 ^1I	+	0.30 $^1S2$	+	0.22 $^1G2$
65	Γ_4	45,484	0.42 ^1F	+	0.30 ^1I	+	0.18 $^1G2$
66	$\Gamma_{2,3}$	45,638	0.48 $^1G2$	+	0.17 $^1G1$	+	0.17 ^1I
67	Γ_4	46,727	0.67 ^1F	+	0.12 $^1D1$	+	0.07 $^1G1$
68	Γ_1	48,344	0.54 $^1G2$	+	0.19 $^1S2$	+	0.09 $^1G1$
69	Γ_4	51,401	0.71 $^1D2$	+	0.08 $^1G1$	+	0.08 ^1F
70	Γ_1	51,481	0.92 ^1F	+	0.06 ^1I	+	0.01 ^3D
71	Γ_4	51,640	0.51 $^1G2$	+	0.41 ^1F	+	0.06 ^1I
72	Γ_1	53,599	0.63 $^3F1$	+	0.19 $^3P1$	+	0.10 ^3H
73	Γ_4	53,659	0.67 $^3F1$	+	0.19 $^3P1$	+	0.11 ^3H
74	$\Gamma_{2,3}$	54,208	0.72 $^3F1$	+	0.13 $^3P1$	+	0.09 ^3H
75	Γ_4	54,282	0.72 $^3F1$	+	0.12 $^3P1$	+	0.09 ^3H
76	Γ_1	57,747	0.50 $^3P1$	+	0.19 $^3F2$	+	0.16 $^3F1$
77	Γ_4	57,871	0.93 $^3F1$	+	0.06 $^3F2$		
78	Γ_4	58,101	0.51 $^3P1$	+	0.18 $^3F2$	+	0.15 $^3F1$
79	$\Gamma_{2,3}$	58,864	0.54 $^3P1$	+	0.16 $^3P2$	+	0.15 $^3F2$
80	Γ_4	59,063	0.53 $^3P1$	+	0.15 $^3P2$	+	0.15 $^3F2$
81	$\Gamma_{2,3}$	60,575	0.68 $^3F1$	+	0.12 ^3D	+	0.08 ^3G
82	Γ_4	60,614	0.70 $^3F1$	+	0.11 ^3G	+	0.10 ^3D
83	Γ_1	60,692	0.70 $^3F1$	+	0.13 ^3G	+	0.08 ^3D
84	Γ_4	60,754	0.69 $^3F1$	+	0.12 ^3D	+	0.08 ^3G
85	Γ_4	64,083	0.77 $^1G1$	+	0.20 ^1I	+	0.02 $^1G2$
86	$\Gamma_{2,3}$	64,145	0.72 $^1G1$	+	0.17 $^1G2$	+	0.07 $^1D2$
87	Γ_1	69,754	0.51 $^1G1$	+	0.24 ^1I	+	0.17 $^1S2$
88	Γ_4	70,343	0.53 $^1G1$	+	0.29 $^1G2$	+	0.10 $^1D2$
89	Γ_4	77,274	0.75 $^1D1$	+	0.11 ^1F	+	0.06 $^1D2$
90	$\Gamma_{2,3}$	80,097	0.83 $^1D1$	+	0.16 $^1D2$		
91	Γ_1	103,295	0.83 $^1S1$	+	0.09 $^1S2$	+	0.08 $^1G1$

[a] *Irreducible representations of the T group, $\Gamma_{2,3} = \Gamma_2 + \Gamma_3$ (degenerate doublets) (G. F. Koster, J. O. Dimmock, R. G. Wheeler, and H. Statz, Properties of the thirty-two point groups, MIT Press, Cambridge, MA (1963)).*

Table 18. Energy levels (cm^{-1}) for Cu^{4+} using the parameters of tables 2 and 4, for Ge site in $Bi_{12}GeO_{20}$, T symmetry, no spin orbit

No.	I.R.[a]	Energy (cm^{-1})	Free ion state
1	Γ_1	0	1.00 ^4F
2	Γ_4	9,490	1.00 ^4F
3	Γ_4	14,930	0.76 ^4F + 0.24 ^4P
4	$\Gamma_{2,3}$	18,807	0.66 ^2G + 0.19 ^2H + 0.14 $^2D2$
5	Γ_4	19,357	0.46 ^2G + 0.34 ^2H + 0.18 ^2P
6	Γ_4	23,777	0.76 ^4P + 0.24 ^4F
7	Γ_4	25,491	0.31 ^2H + 0.29 ^2G + 0.23 $^2D2$
8	Γ_1	26,206	1.00 ^2G
9	Γ_4	28,207	0.51 ^2G + 0.48 ^2H
10	Γ_4	28,786	0.53 ^2H + 0.24 ^2G + 0.23 ^2P
11	$\Gamma_{2,3}$	30,961	0.49 ^2H + 0.44 $^2D2$ + 0.07 $^2D1$
12	Γ_4	32,785	0.43 ^2P + 0.38 ^2H + 0.17 ^2F
13	Γ_4	37,536	0.55 $^2D2$ + 0.26 ^2F + 0.09 ^2G
14	Γ_4	37,953	0.72 ^2H + 0.28 ^2G
15	Γ_1	39,854	1.00 ^2F
16	Γ_4	41,737	0.66 ^2F + 0.12 ^2G + 0.10 ^2H
17	$\Gamma_{2,3}$	43,525	0.40 $^2D2$ + 0.32 ^2G + 0.28 ^2H
18	Γ_4	45,523	0.81 ^2F + 0.16 ^2P + 0.03 ^2H
19	$\Gamma_{2,3}$	64,919	0.91 $^2D1$ + 0.04 ^2H + 0.03 ^2G
20	Γ_4	65,096	0.76 $^2D1$ + 0.16 $^2D2$ + 0.05 ^2F

[a] *Irreducible representations of the T group, $\Gamma_{2,3} = \Gamma_2 + \Gamma_3$ (Bethe notation, G. F. Koster, J. O. Dimmock, R. G. Wheeler, and H. Statz, Properties of the thirty-two point groups, MIT Press, Cambridge, MA (1963)).*

Table 19. Energy levels (cm^{-1}) for Cu^{4+} using the parameters of tables 2 and 4, for Ge site in $Bi_{12}GeO_{20}$, T symmetry, ζ = 1008 cm^{-1}

No.	I.R.[a]	Energy (cm^{-1})	Free ion state
1	$\Gamma_{6,7}$	0	1.00 ^4F
2	$\Gamma_{6,7}$	9,024	0.98 ^4F + 0.01 ^2G
3	Γ_5	9,345	0.99 ^4F + 0.01 ^2G
4	$\Gamma_{6,7}$	9,818	0.99 ^4F
5	Γ_5	10,072	1.00 ^4F
6	Γ_5	14,203	0.81 ^4F + 0.16 ^4P + 0.02 ^2G
7	$\Gamma_{6,7}$	14,782	0.75 ^4F + 0.21 ^4P + 0.02 ^2G
8	Γ_5	15,460	0.69 ^4F + 0.30 ^4P + 0.01 $^2D2$
9	$\Gamma_{6,7}$	15,686	0.69 ^4F + 0.30 ^4P
10	$\Gamma_{6,7}$	18,892	0.62 ^2G + 0.22 ^2H + 0.11 $^2D2$
11	Γ_5	19,255	0.46 ^2G + 0.35 ^2H + 0.14 ^2P
12	$\Gamma_{6,7}$	19,813	0.40 ^2G + 0.29 ^2H + 0.20 ^2P
13	$\Gamma_{6,7}$	23,746	0.69 ^4P + 0.28 ^4F + 0.01 $^2D2$
14	$\Gamma_{6,7}$	23,816	0.73 ^4P + 0.20 ^4F + 0.04 ^2G
15	Γ_5	23,834	0.69 ^4P + 0.30 ^4F
16	Γ_5	24,145	0.79 ^4P + 0.14 ^4F + 0.05 ^2G
17	Γ_5	25,520	0.41 ^2H + 0.22 $^2D2$ + 0.19 ^2G
18	$\Gamma_{6,7}$	25,870	0.40 ^2G + 0.23 ^2H + 0.21 $^2D2$
19	Γ_5	26,782	0.93 ^2G + 0.03 ^4F + 0.02 ^4P
20	$\Gamma_{6,7}$	28,294	0.59 ^2H + 0.38 ^2G + 0.01 $^2D1$
21	Γ_5	28,589	0.57 ^2G + 0.40 ^2H + 0.02 $^2D2$
22	$\Gamma_{6,7}$	29,042	0.55 ^2H + 0.25 ^2G + 0.16 ^2P
23	Γ_5	29,773	0.54 ^2H + 0.25 ^2P + 0.18 ^2G
24	$\Gamma_{6,7}$	31,342	0.48 ^2H + 0.40 $^2D2$ + 0.06 $^2D1$
25	$\Gamma_{6,7}$	33,225	0.40 ^2P + 0.34 ^2H + 0.14 ^2F
26	Γ_5	33,338	0.40 ^2P + 0.38 ^2H + 0.18 ^2F
27	Γ_5	37,543	0.52 $^2D2$ + 0.24 ^2F + 0.10 ^2G
28	$\Gamma_{6,7}$	37,782	0.40 $^2D2$ + 0.25 ^2H + 0.22 ^2F
29	$\Gamma_{6,7}$	38,508	0.54 ^2H + 0.23 ^2G + 0.14 $^2D2$
30	Γ_5	38,664	0.68 ^2H + 0.31 ^2G + 0.01 ^2P
31	Γ_5	40,084	1.00 ^2F
32	$\Gamma_{6,7}$	41,764	0.61 ^2F + 0.11 ^2H + 0.11 ^2G
33	Γ_5	42,706	0.68 ^2F + 0.14 ^2G + 0.07 ^2H
34	$\Gamma_{6,7}$	43,857	0.37 $^2D2$ + 0.30 ^2G + 0.27 ^2H
35	$\Gamma_{6,7}$	45,756	0.76 ^2F + 0.16 ^2P + 0.04 ^2H
36	Γ_5	46,137	0.79 ^2F + 0.17 ^2P + 0.03 ^2H
37	Γ_5	65,145	0.76 $^2D1$ + 0.18 $^2D2$ + 0.04 ^2F
38	$\Gamma_{6,7}$	65,303	0.90 $^2D1$ + 0.04 ^2H + 0.03 $^2D2$
39	$\Gamma_{6,7}$	65,692	0.77 $^2D1$ + 0.14 $^2D2$ + 0.06 ^2F

[a] *Irreducible representations of the double T (cubic) group, $\Gamma_{6,7} = \Gamma_6 + \Gamma_7$ (G. F. Koster, J. O. Dimmock, R. G. Wheeler, and H. Statz, Properties of the thirty-two point groups, MIT Press, Cambridge, MA (1963)).*

Table 20. Energy levels (cm^{-1}) for Zn^{4+} using the parameters of tables 2 and 4, for Ge site in $Bi_{12}GeO_{20}$, T symmetry, no spin orbit

No.	I.R.[a]	Energy (cm^{-1})	Free ion state
1	Γ_4	0	$0.96\ ^3F + 0.04\ ^3P$
2	Γ_4	6,548	$1.00\ ^3F$
3	Γ_1	14,021	$1.00\ ^3F$
4	Γ_4	14,327	$0.73\ ^1D + 0.27\ ^1G$
5	$\Gamma_{2,3}$	14,713	$0.59\ ^1D + 0.41\ ^1G$
6	Γ_4	16,258	$0.96\ ^3P + 0.04\ ^3F$
7	Γ_4	22,686	$0.73\ ^1G + 0.27\ ^1D$
8	Γ_1	24,435	$0.94\ ^1G + 0.06\ ^1S$
9	Γ_4	24,725	$1.00\ ^1G$
10	$\Gamma_{2,3}$	29,774	$0.59\ ^1G + 0.41\ ^1D$
11	Γ_1	56,276	$0.94\ ^1S + 0.06\ ^1G$

Table 21. Energy levels (cm^{-1}) for Zn^{4+} using the parameters of tables 2 and 4, for Ge site in $Bi_{12}GeO_{20}$, T symmetry, $\zeta = 1203\ cm^{-1}$

No.	I.R.[a]	Energy (cm^{-1})	Free ion state
1	Γ_1	0	$0.97\ ^3F + 0.03\ ^3P$
2	Γ_4	699	$0.97\ ^3F + 0.03\ ^3P$
3	$\Gamma_{2,3}$	1,877	$0.96\ ^3F + 0.03\ ^3P$
4	Γ_4	2,325	$0.95\ ^3F + 0.04\ ^3P$
5	Γ_4	8,121	$0.95\ ^3F + 0.03\ ^1D + 0.01\ ^1G$
6	Γ_4	8,182	$1.00\ ^3F$
7	$\Gamma_{2,3}$	8,525	$0.98\ ^3F + 0.01\ ^1D + 0.01\ ^3P$
8	Γ_1	8,926	$1.00\ ^3F$
9	Γ_4	15,124	$0.40\ ^1D + 0.39\ ^3F + 0.15\ ^3P$
10	$\Gamma_{2,3}$	15,327	$0.39\ ^1D + 0.39\ ^3P + 0.22\ ^1G$
11	Γ_4	16,486	$0.65\ ^3F + 0.17\ ^3P + 0.10\ ^1D$
12	Γ_4	18,312	$0.62\ ^3P + 0.19\ ^1D + 0.16\ ^1G$
13	Γ_4	18,589	$0.97\ ^3P + 0.03\ ^3F$
14	$\Gamma_{2,3}$	18,701	$0.57\ ^3P + 0.20\ ^1G + 0.18\ ^1D$
15	Γ_1	18,903	$0.96\ ^3P + 0.03\ ^3F + 0.01\ ^1S$
16	Γ_4	24,734	$0.69\ ^1G + 0.28\ ^1D + 0.02\ ^3F$
17	Γ_1	26,307	$0.94\ ^1G + 0.05\ ^1S + 0.01\ ^3P$
18	Γ_4	26,565	$1.00\ ^1G$
19	$\Gamma_{2,3}$	31,744	$0.58\ ^1G + 0.41\ ^1D + 0.01\ ^3P$
20	Γ_1	58,264	$0.94\ ^1S + 0.06\ ^1G + 0.01\ ^3P$

[a] *Irreducible representations of the T group, $\Gamma_{2,3} = \Gamma_2 + \Gamma_3$ (degenerate doublets) (G. F. Koster, J. O. Dimmock, R. G. Wheeler, and H. Statz, Properties of the thirty-two point groups, MIT Press, Cambridge, MA (1963)).*

Table 22. Energy levels (cm^{-1}) for Ga^{4+} using the parameters of tables 2 and 4, for Ge site in $Bi_{12}GeO_{20}$, T symmetry, no spin orbit

No.	I.R.[a]	Energy (cm^{-1})	Free ion state
1	Γ_4	0	$1.00\ ^2D$
2	$\Gamma_{2,3}$	4,981	$1.00\ ^2D$

[a]*Irreducible representations of the T (cubic) group, $\Gamma_{2,3} = \Gamma_2 + \Gamma_3$ (Bethe notation, G. F. Koster, J. O. Dimmock, R. G. Wheeler, and H. Statz, Properties of the thirty-two point groups, MIT Press, Cambridge, MA (1963)).*

Table 23, Energy levels (cm^{-1}) for Ga^{4+} using the parameters of tables 2 and 4, for Ge site in $Bi_{12}GeO_{20}$, T symmetry, $\zeta = 1496\ cm^{-1}$

No.	I.R.[a]	Energy (cm^{-1})	Free ion state
1	Γ_5	0	$1.00\ ^2D$
2	$\Gamma_{6,7}$	1,561	$1.00\ ^2D$
3	$\Gamma_{6,7}$	7,160	$1.00\ ^2D$

[a]*Irreducible representations of the double T (cubic) group, $\Gamma_{6,7} = \Gamma_6 + \Gamma_7$ (G. F. Koster, J. O. Dimmock, R. G. Wheeler, and H. Statz, Properties of the thirty-two point groups, MIT Press, Cambridge, MA (1963)).*

6. Conclusion

The crystallographic data on six host materials have been used to find the crystal-field components at sites that could be occupied by quadruply ionized transition-metal ions with the $3d^N$ electronic configuration. Using approximate values for the effective radial integrals ρ_2 and ρ_4, we obtain the crystal-field parameters, B_{kq}, for Cr^{4+} in the host crystals $NaTiSiO_5$, Y_2SiBeO_7, $Bi_4Si_3O_{12}$, and $Bi_4Ge_3O_{12}$, assuming that the Cr^{4+} ion occupied the Ge, Ti, or Si site in these crystals.

For the host crystal $Bi_{12}GeO_{20}$ the Ge site has the cubic group symmetry T, and the entire quadruply ionized $3d^N$ series energy levels were calculated using estimated crystal-field parameters. The calculated energy levels are for $\zeta = 0$ and for the value of ζ corresponding to the free-ion results. Experimental values of several energy levels for Cr^{4+} have been reported and upon comparison with the results obtained here, our estimated crystal-field parameters are too large. More experimental data are needed to ascertain whether this difference is significant.

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Appendix A.—Crystallographic and X-Ray Data

Appendix A

Contents

The following tables give the crystallographic and x-ray data on each of the compounds considered. The crystal-field components, A_{kq}, are calculated for the monopole (point-charge), self-induced, and dipole contributions. Following each table is a list of references for that particular compound. These references include such topics as crystal growth, index of refraction, and electron spin resonance investigations. However, the list of references is not, in any sense, exhaustive and if further investigations are contemplated on any compound, additional library searches should be undertaken.

A-1. Na_2TiSiO_5

A-1.1 Crystallographic Data on Na_2TiSiO_5

Tetragonal (*P4/nmm*), 129, $Z = 2$[a]

Ion	Site	Symmetry	x[b]	y	z	q	α (Å^3)[c]
Ti	2*c*	C_{4v}	1/2	0	0.9343	4	0.506
Na	4*e*	C_{2h}	1/4	1/4	1/2	1	0.147
Si	2*a*	D_{2d}	0	0	0	4	0.0165
O_1	8*i*	C_s	0	0.2071	0.1831	–2	1.349
O_2	2*c*	C_{4v}	1/2	0	–0.7338	–2	1.349

[a] *N. F. M. Henry and K. Lonsdale, International tables for x-ray crystallography, Vol. I: Symmetry groups, Kynoch, Birmingham, UK (1969).*
[b] *X-ray data: a = 6.480 Å, c = 5.107 Å (Nyman et al (1978)).*
[c] *Schmidt et al (1979).*

A-1.2 Crystal-Field Components, A_{kq} (cm^{-1}/Å^k) for the Si (D_{2d}) Site in Na_2TiSiO_5

A_{kq}	Monopole	Self-induced	Dipole	Total
A_{20}	7,285	548.7	–34,349	–26,515
A_{32}	–64,975	25,258	–48,610	–88,327
A_{40}	–31,427	19,391	–20,545	–32,581
A_{44}	17,004	–12,063	21,554	26,494
A_{52}	326.3	–628.4	9,042	8,740

A-1.3 Crystal-Field Components, A_{kq} (cm^{-1}/Å^k), for the Ti (C_{4v}) Site in Na_2TiSiO_5

A_{kq}	Monopole	Self-induced	Dipole	Total
A_{10}	15,041	0	114,675	129,716
A_{20}	18,952	–2,906	38,432	54,478
A_{30}	48,794	–13,854	36,992	71,932
A_{40}	18,057	–10,303	42,160	49,914
A_{44}	10,890	–4,552	766.4	7,105
A_{50}	4,284	–5,673	25,232	23,843
A_{54}	–6,132	3,088	2,933	–111.3

A-1.4 Na_2TiSiO_5 References

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A-2. $Y_2SiBe_2O_7$

A-2.1 Crystallographic Data on $Y_2SiBe_2O_7$

Tetragonal D_{3d}^3 ($P\bar{4}2_1m$), 113, $Z = 2$

Ion	Site	Symmetry	x^a	y	z	q	α (Å^3)^b
Y	4*e*	C_s	0.1595	0.6595	0.4873	3	0.870
Si	2*a*	S_4	0	0	0	4	0.0165[c]
Be	4*e*	C_s	0.363	0.863	0.031	2	0.0125
O_1	8*f*	C_1	0.0823	0.1664	0.7928	–2	1.349
O_2	4*e*	C_2	0.3561	0.8561	0.7053	–2	1.349
O_3	2*c*	C_{2v}	0	1/2	0.8275	–2	1.349

[a] *X-ray data: $a = 7.283$ Å; $c = 4.755$ Å, Bartram (1969).*
[b] *Schmidt et al (1979).*
[c] *Tessman et al (1953).*

A-2.2 Crystal-Field Components, A_{kq} (cm^{-1}/Å^k), for the Si Site (S_4) in $Y_2SiBe_2O_7$

A_{kq}	Monopole	Self-induced	Dipole	Total
A_{20}	10,029	–468.9	–19,678	–10,118
$\mathrm{Re}A_{32}$	35,565	–12,974	26,656	49,247
$\mathrm{Im}A_{32}$	–46,373	17,029	–40,428	–69,772
A_{40}	–28,792	16,971	–23,527	–35,348
$\mathrm{Re}A_{44}$	–4,073	2,468	–6,484	–8,089
$\mathrm{Im}A_{44}$	–14,462	9,193	–17,375	–22,644
$\mathrm{Re}A_{52}$	902.0	–662.1	–2,652	–2,412
$\mathrm{Im}A_{52}$	–1,164	866.0	3,394	3,096
$\lvert A_{44}\rvert$	15,025	—	—	24,045

A-2.3 $Y_2SiBe_2O_7$ References

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A-3. $Bi_4X_3O_{12}$ (X = Si, Ge)

A-3.1 Crystallographic Data on $Bi_4X_3O_{12}$

Cubic $T_d^6(I\bar{4}3d)$, 220, $Z = 4$

Ion	Site	Symmetry	x^a	y	z	q	α (Å^3)
Bi	16*c*	C_3	x	x	x	3	2.23[a]
X	12*a*	S_4	0	1/4	3/8	4	α_x[a]
O	48*e*	C_1	x	y	z	–4	1.349[b]

[a] *Fraga et al (1976), $\alpha_{Si} = 0.03$ (Å^3), $\alpha_{Ge} = 0.12$ (Å^3).*
[b] *Schmidt et al (1979).*

A-3.2 X-Ray Data on $Bi_4X_3O_{12}$

X	a	x_{Bi}	x_0	y_0	z_0
Si	10.300[a]	0.0857	0.0607	0.1335	0.2875
Ge	10.513[b]	0.0876	0.0689	0.1277	0.2875

[a] *Wyckoff (1968), Vol. 4.*
[b] *Fisher and Waldner (1982).*

A-3.3 Crystal-Field Components, A_{kq} (cm^{-1}/Å^k), for the Si Site (S_4) of $Bi_4Si_3O_{12}$

A_{kq}	Monopole	Self-induced	Dipole	Total
A_{20}	–4,423	1,103	11,851	8,531
ReA_{32}	39,156	–15,088	35,345	59,414
ImA_{32}	55,809	–21,662	43,774	77,921
A_{40}	–29,886	19,317	–36,749	–47,317
ReA_{44}	–7,631	4,551	–3,239	–6,319
ImA_{44}	18,425	–12,613	15,697	21,509
ReA_{52}	–2,043	1,506	2,727	2,190
ImA_{52}	–2,628	2,150	3,917	3,439
$\lvert A_{44}\rvert$	19,943	—	—	22,418

A-3.4 Crystal-Field Components, A_{kq} ($cm^{-1}/Å^k$), for the Ge Site (S_4) of $Bi_4Ge_3O_{12}$

A_{kq}	Monopole	Self-induced	Dipole	Total
A_{20}	-9,149	1,563	7,098	-488.4
ReA_{32}	26,496	-8,445	21,045	39,096
ImA_{32}	43,745	-14,017	29,123	58,851
A_{40}	-19,352	10,242	-22,771	-31,881
ReA_{44}	-7,790	3,872	-2,562	-6,480
ImA_{44}	13,318	-7,527	8,938	14,729
ReA_{52}	-2,366	1,523	1,117	274.0
ImA_{52}	-3,549	2,507	1,981	938.8
$\lvert A_{44}\rvert$	15,429	—	—	16,091

A-3.5 $Bi_4X_3O_{12}$ References

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A-4. $Bi_{12}XO_{20}$ (X = Ge, Si)

A-4.1 Crystallographic Data on $Bi_{12}XO_{20}$

Cubic T^3 ($I23$), 197, $Z = 2$

Ion	Site	Symmetry	x	y	z	q	α (Å^3)
Bi	24*f*	C_1	x	y	z	3	2.23[a]
X	2*a*	T	0	0	0	4	α_x[a]
O_1	24*f*	C_1	x	y	z	–2	1.349[b]
O_2	8*c*	C_3	x	x	x	–2	1.349
O_3	8*c*	C_3	x	x	x	–2	1.349

[a]*Fraga et al (1976).*
[b]*Schmidt et al (1979).*

A-4.2 X-Ray Data on $Bi_{12}XO_{20}$

X	a	x_{Bi}	y_{Bi}	z_{Bi}	x_{O1}	y_{O1}	z_{O1}
Ge	10.1455[a]	0.82409	0.68158	0.98433	0.8655	0.7477	0.5145
Si	10.10433[b]	0.17564	0.31741	0.01592	0.1348	0.2523	0.4858

X	x_{O2}	x_{O3}	α_x (Å^3)[c]
Ge	0.8019	0.0977	0.12
Si	0.1950	0.9059	0.03

[a]*Abrahams et al (1967).*
[b]*Abrahams et al (1979).*
[c]*Fraga et al (1976).*

A-4.3 Crystal-Field Components, A_{kq} (cm^{-1}/Å^k), for the Ge Site of $Bi_{12}GeO_{20}$[a]

A_{kq}	Monopole	Self-induced	Dipole	Total
A_{32}	*i*54,550	–*i*17,875	*i*50,303	86,978
A_{40}	–25,350	13,407	–26,296	–38,240
A_{60}	4,766.4	–5,328.1	7,328.2	6,766.5
A_{62}	163.03	17.182	–35.978	144.24
A_{72}	–*i*3,901.1	*i*5,796.2	–*i*6,963.0	–*i*5,067.9

[a] $A_{44} = \sqrt{\frac{5}{14}}\,A_{40}$, $A_{64} = -\sqrt{\frac{7}{2}}\,A_{60}$, $A_{66} = -\sqrt{\frac{5}{11}}\,A_{62}$, *and* $A_{76} = \sqrt{\frac{11}{13}}\,A_{72}$.

A-4.4 Crystal-Field Components, A_{kq} ($cm^{-1}/Å^k$), for the Si Site (T) of $Bi_{12}SiO_{20}$[a]

A_{kq}	Monopole	Self-induced	Dipole	Total
A_{32}	$-i64{,}514$	$i23{,}949$	$-i64{,}411$	$-i104{,}976$
A_{40}	−31,029	18,698	−35,224	−47,555
A_{60}	6,361.3	−8,079.2	10,613	8,895.5
A_{62}	170.64	18.406	−35.384	153.67
A_{72}	$i5{,}446.7$	$-i9{,}160.9$	$i10{,}524$	$i6{,}810.0$

[a] $A_{44} = \sqrt{\frac{5}{14}}\,A_{40}$, $A_{64} = -\sqrt{\frac{7}{2}}\,A_{60}$, $A_{66} = -\sqrt{\frac{5}{11}}\,A_{62}$, and $A_{76} = \sqrt{\frac{11}{13}}\,A_{72}$.

A-4.5 $Bi_{12}XO_{20}$ (X = Ge, Si) References

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